Kwantumfysica I

2008-2009

Hoorcollege vrijdag 5 december 2008

Vragen?

Extra leestof / achtergrond materiaal uit Cohen-Tannoudji boek

Quantum Mechanics (Volume 1 en 2)
Claude Cohen-Tannoudji *et al.*

<u>Zeer goed boek</u> – sluit goed aan op Liboff

Zeer goed naslag werk
Alles goed geïntroduceerd, onderbouwd en afgeleid

Vandaag uitgedeeld:

Appendix 1	Fourier transformations
Appendix 2	Dirac delta functions
Appendix 3	Lagrangian and Hamiltonian classical mechanics

Vandaag:

Kleine rekenvoorbeeldjes over begrippen en formalisme

Met meer / nieuw

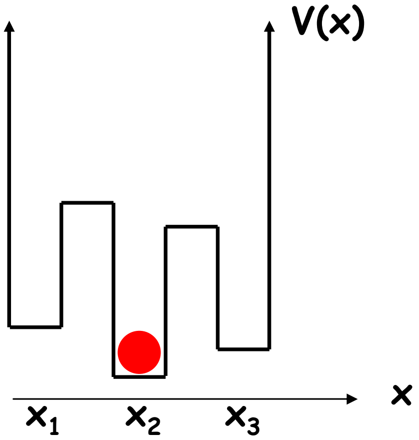
1. Basis / representatie veranderen
2. Commutators

Rekenvoorbeeldjes met zeer simpele discrete systemen:
Gedanken experiments

Gebruikt alleen 2 x 2 of 3 x 3 discrete matrices voor operatoren

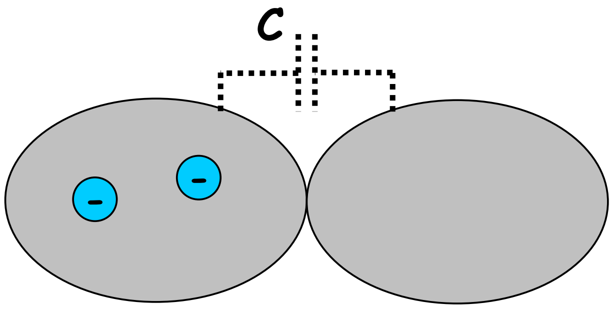
Toestanden zijn dan vectoren met 2 of 3 elementen

Mechanisch systeem, met 3 toestanden



Positie toestanden $|x_1\rangle, |x_2\rangle, |x_3\rangle$ vormen geschikte basis

Ander modelsysteempje met 3 toestanden:
Neutraal geladen, twee zwak gekoppelde geleidende eilandjes
(neem aan dat de lading van het geheel neutraal is)



N_{left} = -1, 0 of +1

$Q_C = N_{left}\, e$

$E_{elec} = (Q_C)^2/2C$

Ladings-toestanden $|N_{left}=-1\rangle$, $|N_{left}=0\rangle$, $|N_{left}=1\rangle$ vormen geschikte basis

Matrix en vector representatie in deze basis:

$$\hat{N}_{left} \leftrightarrow \begin{pmatrix} -1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

$$\left|N_{left}=-1\right\rangle = \left|-1\right\rangle \leftrightarrow \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \qquad \left|N_{left}=0\right\rangle = \left|0\right\rangle \leftrightarrow \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \qquad \left|N_{left}=1\right\rangle = \left|1\right\rangle \leftrightarrow \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$$

Superposition state

$$|\Psi\rangle = \frac{|-1\rangle + i|1\rangle}{\sqrt{2}} \quad \leftrightarrow \quad \begin{pmatrix} \frac{1}{\sqrt{2}} \\ 0 \\ i\frac{1}{\sqrt{2}} \end{pmatrix}$$

Expectation value

Uncertainty

Time evolution

Postulaat 4

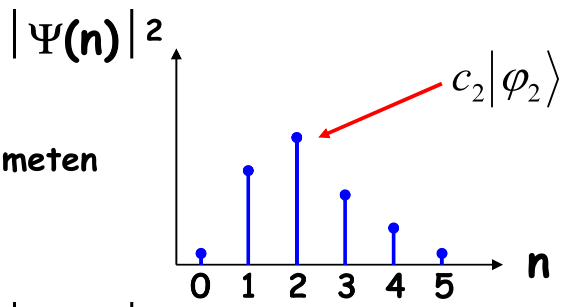
Meting van eigenschap A geeft altijd een eigenwaarde van Â.
Is het resultaat a, dan is de toestand na het meten is de bijbehorende eigenfunctie φ_a.

$$\hat{N}|\varphi_n\rangle = n|\varphi_n\rangle$$

$$\hat{A}|\varphi_n\rangle = n^2|\varphi_n\rangle$$

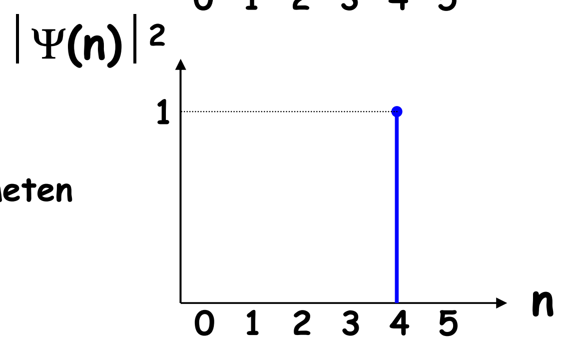
Discreet voorbeeld A=N²

Voor meten



$$\Psi(n) = c_n = \langle \varphi_n | \Psi \rangle$$

Na meten



Meetuikomst was 16

$$\Rightarrow |\Psi\rangle = |\varphi_4\rangle$$

Hier notatie als in week 2 van colleges

Postulaat 5 - discreet (weinig aandacht in boek)

Kans op meetuitkomst a is $\left|\Sigma\ \Psi(n,t)^*\ \varphi_a(n)\right|^2$

|Inwendig product $\Psi(n,t)^*$ en $\varphi_a(n)$ $|^2$

Zelfde voorbeeld $A=N^2$

N.B. in dit voorbeeld (vorige slide), vallen de eigenvectoren $\varphi_a(n)$ samen met de basisvectoren die horen bij de coordinaten n. Algemene geval komt hierna.

Stel voor het meten

$$\Psi(n) = 0\,\varphi_0(n) + c_1\varphi_1(n) + c_2\varphi_2(n) + 0\,\varphi_3(n) + c_4\varphi_4(n) + 0\,\varphi_5(n)$$

$$\Psi(n) = \sum_n c_n\varphi_n(n) \qquad \text{met} \qquad \sum_n c_n^* c_n = 1$$

Kans op meetuitkomst 16 is dan

$$\left|\sum_n \Psi(n)^*\varphi_4(n)\right|^2 = \left|\sum_n c_n^*\varphi_n^*(n)\cdot\varphi_4(n)\right|^2 = \left|c_4\right|^2$$

Hier notatie als in week 2 van colleges

Vervolg Postulaat 5 – discreet

In het algemeen, hoeven de eigenvectoren $\varphi_a(n)$ niet samen te vallen met de basisvectoren die worden gebruikt in de somaties over coordinaten n in onderstaande voorbeeld. Dit maakt de link met het continue geval (volgende slide) duidelijker.

Stel voor het meten

$$\Psi(n) = 0\,\varphi_0(n) + c_1\varphi_1(n) + c_2\varphi_2(n) + 0\,\varphi_3(n) + c_4\varphi_4(n) + 0\,\varphi_5(n)$$

$$\Psi(n) = \sum_m c_m\varphi_m(n) \qquad \text{met} \qquad \sum_m c_m^* c_m = 1$$

Kans op meetuitkomst behorend bij eigenvector $\varphi_4(n)$ is dan

$$\left|\sum_n \Psi(n)^*\varphi_4(n)\right|^2 = \left|\sum_n\left(\sum_m c_m^*\varphi_m^*(n)\right)\cdot\varphi_4(n)\right|^2 =$$

$$0 + \left|\sum_n c_1^*\varphi_1^*(n)\cdot\varphi_4(n)\right|^2 + \left|\sum_n c_2^*\varphi_2^*(n)\cdot\varphi_4(n)\right|^2 + 0 + \left|\sum_n c_4^*\varphi_4^*(n)\cdot\varphi_4(n)\right|^2 + 0 =$$

$$0+0+0+0+\left|c_4^*\right|^2 + 0 = \left|c_4\right|^2$$

Hier Dirac notatie

Postulaat 5 - discreet (weinig aandacht in boek)

Kans op meetuitkomst a is $\left|\langle\Psi(t)|\varphi_a\rangle\right|^2$ ← |Inwendig product $\Psi(n,t)^*$ en $\varphi_a(n)$ $|^2$

Zelfde voorbeeld $A=N^2$

Stel voor het meten $|\Psi\rangle = c_1|\varphi_1\rangle + c_2|\varphi_2\rangle + c_4|\varphi_4\rangle$

$$\sum_m c_m^* c_m = 1$$

Kans op meetuitkomst 16 is $\left|\langle\Psi|\varphi_4\rangle\right|^2$

$$\left|\langle\Psi|\varphi_4\rangle\right|^2 = \left|c_1^*\langle\varphi_1|\varphi_4\rangle\right|^2 + \left|c_2^*\langle\varphi_2|\varphi_4\rangle\right|^2 + \left|c_4^*\langle\varphi_4|\varphi_4\rangle\right|^2 = |c_4|^2$$

Voor willekeurige $\Psi(n)$ de c_m bepalen: $c_m = \langle\varphi_m|\Psi\rangle$

⇒ Spectrale decompositie

Vorige slide geschreven als vectoren
(hier over het interval n=0..4, daarbuiten zijn alle c_n=0):

$$\langle\Psi| \leftrightarrow \begin{pmatrix} 0 & c_1^* & c_2^* & 0 & c_4^* \end{pmatrix} \qquad |\varphi_4\rangle \leftrightarrow \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}$$

$$\left|\langle\Psi|\varphi_4\rangle\right|^2 \leftrightarrow \left| \begin{pmatrix} 0 & c_1^* & c_2^* & 0 & c_4^* \end{pmatrix} \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 1 \end{pmatrix} \right|^2 = |c_4|^2$$

N.B. in het voorbeeld op deze slide (zie ook vorige slides), vallen de eigenvectoren $\varphi_a(n)$ samen met de basisvectoren die horen bij de coordinaten n.

Finding eigenvalues, eigenvectors, eigenvalue equations of type $\hat{H}|\varphi\rangle = E|\varphi\rangle$

How many eigenvalues, what are they?

$$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 3 \end{pmatrix} \Rightarrow \quad 1,\ 2,\ 3$$

How many eigenvectors, what are they (normalized)?

$$\begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$$

How to find these in general? $\hat{H}|\varphi_i\rangle = E_i|\varphi_i\rangle$

$$\begin{pmatrix} V_1 & 0 & 0 \\ 0 & V_2 & 0 \\ 0 & 0 & V_3 \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \\ c_3 \end{pmatrix}_i = E_i \begin{pmatrix} c_1 \\ c_2 \\ c_3 \end{pmatrix}_i$$

represented in certain basis (x_i or N_{left} in previous examples)

Look up linear algebra:

$$\begin{vmatrix} V_1 - E_i & 0 & 0 \\ 0 & V_2 - E_i & 0 \\ 0 & 0 & V_3 - E_i \end{vmatrix} = 0$$

$$(V_1 - E_i)(V_2 - E_i)(V_3 - E_i) = 0$$

$$E_{1,2,3} = V_1, V_2, V_3$$

For the eigenvectors,solve

$$\begin{pmatrix} V_1 & 0 & 0 \\ 0 & V_2 & 0 \\ 0 & 0 & V_3 \end{pmatrix}\begin{pmatrix} c_1 \\ c_2 \\ c_3 \end{pmatrix}_i = E_i\begin{pmatrix} c_1 \\ c_2 \\ c_3 \end{pmatrix}_i \qquad \Rightarrow \qquad \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$$

Dirac notation, normalized states, orthogonality

$$|\varphi_1\rangle \leftrightarrow \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \qquad |\varphi_2\rangle \leftrightarrow \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \qquad |\varphi_3\rangle \leftrightarrow \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$$

$$\begin{pmatrix} 1 & 0 & 0 \end{pmatrix}\begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} = 1$$

$$\begin{pmatrix} 1 & 0 & 0 \end{pmatrix}\begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} = 0$$

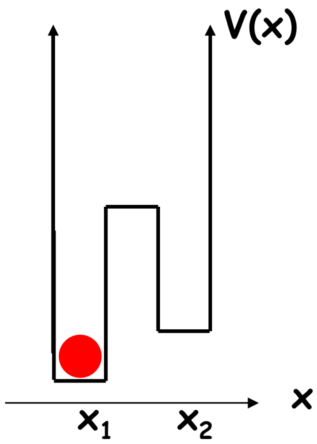
A bit less obvious to solve $\hat{H} = \hat{H}_V + \hat{H}_T \leftrightarrow \begin{pmatrix} V_1 & T \\ T & V_2 \end{pmatrix} = \begin{pmatrix} V_1 & 0 \\ 0 & V_2 \end{pmatrix} + \begin{pmatrix} 0 & T \\ T & 0 \end{pmatrix}$

but more interesting: OFF-DIAGONAL ELEMENTS

V_i beschrijft de energie van het systeem op plaats x_i

T beschrijft de energie van het mechanisme dat overgangen van 1 naar 2 en vice versa mogelijk maakt.

Mechanisch systeem, met 2 toestanden



$$\hat{H} = \hat{H}_V + \hat{H}_T \leftrightarrow \begin{pmatrix} V_1 & T \\ T & V_2 \end{pmatrix} = \begin{pmatrix} V_1 & 0 \\ 0 & V_2 \end{pmatrix} + \begin{pmatrix} 0 & T \\ T & 0 \end{pmatrix}$$

$$\begin{pmatrix} V_1 & T \\ T & V_2 \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \end{pmatrix}_i = E_i \begin{pmatrix} c_1 \\ c_2 \end{pmatrix}_i \qquad \Rightarrow$$

$$\begin{cases} E_1 = \dfrac{V_1 + V_2}{2} - \dfrac{1}{2}\sqrt{(V_1 - V_2)^2 + 4T^2} \\ E_2 = \dfrac{V_1 + V_2}{2} + \dfrac{1}{2}\sqrt{(V_1 - V_2)^2 + 4T^2} \end{cases} \quad \begin{pmatrix} \text{the choice of } + \text{ and } - \text{ here assumes} \\ V_1 < V_2 \text{ and } T < 0, \text{and } T \text{ a real number.} \end{pmatrix}$$

$$\begin{pmatrix} c_1 \\ c_2 \end{pmatrix}_1 = \begin{pmatrix} \cos\left(\dfrac{\theta}{2}\right) \\ \sin\left(\dfrac{\theta}{2}\right) \end{pmatrix}, \qquad \begin{pmatrix} c_1 \\ c_2 \end{pmatrix}_2 = \begin{pmatrix} -\sin\left(\dfrac{\theta}{2}\right) \\ \cos\left(\dfrac{\theta}{2}\right) \end{pmatrix} \quad \text{with} \quad \tan\theta = \frac{2T}{V_1 - V_2}$$

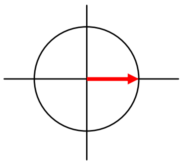
$$0 \le \theta < \pi$$

$$\hat{H} = \hat{H}_V + \hat{H}_T \leftrightarrow \begin{pmatrix} V_1 & T \\ T & V_2 \end{pmatrix} = \begin{pmatrix} V_1 & 0 \\ 0 & V_2 \end{pmatrix} + \begin{pmatrix} 0 & T \\ T & 0 \end{pmatrix}$$

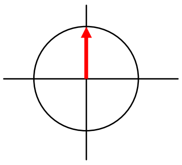
$T = 0 \quad \Rightarrow \quad \theta = 0$

$$\begin{cases} E_1 = V_1 \\ E_2 = V_2 \end{cases}$$

$$\begin{pmatrix} c_1 \\ c_2 \end{pmatrix}_1 = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$



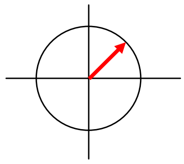
$$\begin{pmatrix} c_1 \\ c_2 \end{pmatrix}_2 = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$



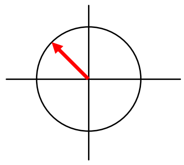
$V_1 = 0, \quad V_2 = 0 \quad \Rightarrow \quad \theta = \pi / 2$

$$\begin{cases} E_1 = -T \\ E_2 = +T \end{cases}$$

$$\begin{pmatrix} c_1 \\ c_2 \end{pmatrix}_1 = \begin{pmatrix} 1/\sqrt{2} \\ 1/\sqrt{2} \end{pmatrix}$$



$$\begin{pmatrix} c_1 \\ c_2 \end{pmatrix}_2 = \begin{pmatrix} -1/\sqrt{2} \\ 1/\sqrt{2} \end{pmatrix}$$



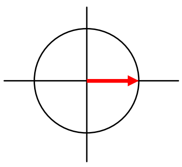
What about changing to the basis compatible with T?

$$\hat{H} = \hat{H}_V + \hat{H}_T \leftrightarrow \begin{pmatrix} V_1 & T \\ T & V_2 \end{pmatrix}^{VB} = \begin{pmatrix} V_1 & 0 \\ 0 & V_2 \end{pmatrix}^{VB} + \begin{pmatrix} 0 & T \\ T & 0 \end{pmatrix}^{VB}$$

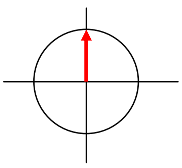
$T = 0 \quad \Rightarrow$

$$\begin{cases} E_1 = V_1 \\ E_2 = V_2 \end{cases}$$

$$\begin{pmatrix} c_1 \\ c_2 \end{pmatrix}_1 = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$



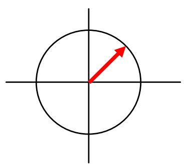
$$\begin{pmatrix} c_1 \\ c_2 \end{pmatrix}_2 = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$



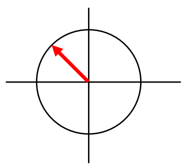
$V_1 = 0, \quad V_2 = 0 \quad \Rightarrow$

$$\begin{cases} E_1 = -T \\ E_2 = +T \end{cases}$$

$$\begin{pmatrix} c_1 \\ c_2 \end{pmatrix}_1 = \begin{pmatrix} 1/\sqrt{2} \\ 1/\sqrt{2} \end{pmatrix}$$



$$\begin{pmatrix} c_1 \\ c_2 \end{pmatrix}_2 = \begin{pmatrix} -1/\sqrt{2} \\ 1/\sqrt{2} \end{pmatrix}$$



$$\hat{R} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix} \qquad \hat{R}^{-1} = \hat{R}^{+} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix}, \qquad \hat{R}^{+}\hat{R} = \hat{R}\hat{R}^{+} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

This rotation operation is in fact a very simple Fourier transform

What about changing to the basis compatible with T?

$$\hat{H} = \hat{H}_V + \hat{H}_T \leftrightarrow \begin{pmatrix} V_1 & T \\ T & V_2 \end{pmatrix}^{VB} = \begin{pmatrix} V_1 & 0 \\ 0 & V_2 \end{pmatrix}^{VB} + \begin{pmatrix} 0 & T \\ T & 0 \end{pmatrix}^{VB}$$

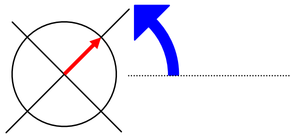
$$\hat{H}_T^{TB} \leftrightarrow \hat{R}^{+} \begin{pmatrix} 0 & T \\ T & 0 \end{pmatrix}^{VB} \hat{R} = \begin{pmatrix} -T & 0 \\ 0 & T \end{pmatrix}^{TB}$$

$$\hat{H}_V^{TB} \leftrightarrow \hat{R}^{+} \begin{pmatrix} V_1 & 0 \\ 0 & V_2 \end{pmatrix}^{VB} \hat{R} = \begin{pmatrix} \frac{V_1+V_2}{2} & \frac{V_1-V_2}{2} \\ \frac{V_1-V_2}{2} & \frac{V_1+V_2}{2} \end{pmatrix}^{TB}$$

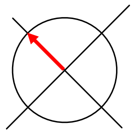
$V_1 = 0, \quad V_2 = 0 \quad \Rightarrow$

$$\begin{cases} E_1 = -T \\ E_2 = +T \end{cases}$$

$$\hat{R}\begin{pmatrix} 1/\sqrt{2} \\ 1/\sqrt{2} \end{pmatrix}^{VB} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}^{TB}$$



$$\hat{R}\begin{pmatrix} -1/\sqrt{2} \\ 1/\sqrt{2} \end{pmatrix}^{VB} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}^{TB}$$



$$\hat{R} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix} \qquad \hat{R}^{-1} = \hat{R}^{+} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix}, \qquad \hat{R}^{+}\hat{R} = \hat{R}\hat{R}^{+} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

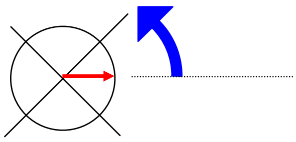
What are the old V-basis vectors in this T basis?

$$\hat{H} = \hat{H}_V + \hat{H}_T \leftrightarrow \begin{pmatrix} V_1 & T \\ T & V_2 \end{pmatrix}^{VB} = \begin{pmatrix} V_1 & 0 \\ 0 & V_2 \end{pmatrix}^{VB} + \begin{pmatrix} 0 & T \\ T & 0 \end{pmatrix}^{VB}$$

$T = 0 \quad \Rightarrow$

$$\begin{cases} E_1 = V_1 \\ E_2 = V_2 \end{cases}$$

$$\hat{R}\begin{pmatrix} 1 \\ 0 \end{pmatrix}^{VB} = \begin{pmatrix} 1/\sqrt{2} \\ -1/\sqrt{2} \end{pmatrix}^{TB}$$



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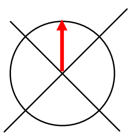
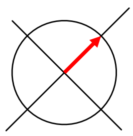


$V_1 = 0, \quad V_2 = 0 \quad \Rightarrow$

$$\begin{cases} E_1 = -T \\ E_2 = +T \end{cases}$$

$$\hat{R}\begin{pmatrix} 1/\sqrt{2} \\ 1/\sqrt{2} \end{pmatrix}^{VB} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}^{TB}$$



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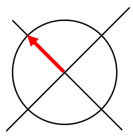

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Now let's go through this again, and measure the T and V properties

Commutator bracket: (H5 p. 130)

$\left[\hat{A},\hat{B}\right]=\hat{A}\hat{B}-\hat{B}\hat{A}$ **Commutator (in general an operator)**

$\left[\hat{A},\hat{B}\right]=0$ $\hat{A}$ **and** $\hat{B}$ **commute, same eigenvectors**

$\left[\hat{x},\hat{p}_x\right]=i\hbar\cdot\hat{I} \quad \Rightarrow \quad \Delta x\Delta p_x>\hbar/2$

$$\hat{H}_V\hat{H}_T \leftrightarrow \begin{pmatrix} V_1 & 0 \\ 0 & V_2 \end{pmatrix}\begin{pmatrix} 0 & T \\ T & 0 \end{pmatrix}=\begin{pmatrix} 0 & V_1T \\ V_2T & 0 \end{pmatrix}$$

$$\hat{H}_T\hat{H}_V \leftrightarrow \begin{pmatrix} 0 & T \\ T & 0 \end{pmatrix}\begin{pmatrix} V_1 & 0 \\ 0 & V_2 \end{pmatrix}=\begin{pmatrix} 0 & V_2T \\ V_1T & 0 \end{pmatrix}$$

$$f\left(\hat{H}_V\right)=f\left(\begin{pmatrix} V_1 & 0 \\ 0 & V_2 \end{pmatrix}\right)=\begin{pmatrix} g_1(V_1,V_2) & 0 \\ 0 & g_2(V_1,V_2) \end{pmatrix}$$

Commutator bracket:

$\left[\hat{A},\hat{B}\right]=\hat{A}\hat{B}-\hat{B}\hat{A}$ **Commutator (in general an operator)**

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$\left[\hat{x},\hat{p}_x\right]=i\hbar\cdot\hat{I} \quad \Rightarrow \quad \Delta x\Delta p_x > \hbar/2$

Measure A with result a_1, then B, then again A

$\Rightarrow$ $\hat{A}$ **and** $\hat{B}$ **commute, measurement gives again result a_1**

$\Rightarrow$ $\hat{A}$ **and** $\hat{B}$ **do not commute, gives arbitrary outcome**

Samenvatting:

1. Commutators
2. Kleine rekenvoorbeeldjes over veel begrippen

Volgende week: H6

Afmaken deze week

-ontaarding (degeneracy)

-C.S.C.O – Hilbert space basis

More on time evolution

Conservation laws

Parity