Kwantumfysica I

2008-2009

Hoorcollege dinsdag 9 december 2008

Deze week Hoofdstuk 6

Vragen n.a.v. stof vorige week of werkcollege?

Extra leestof / achtergrond materiaal uit Cohen-Tannoudji boek

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

Zeer goed boek – sluit goed aan op Liboff

Zeer goed naslag werk
Alles goed geïntroduceerd, onderbouwd en afgeleid

Vandaag uitgedeeld:

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

Vandaag:

1. Afmaken vorige week

   - Commutators

   - Degenaracy (ontaarding)

   - C.S.C.O. (volgend college)

2. Meer over tijdsevoluties en Fourier

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)

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

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

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

Degenerate (ontaarde) states

How to find eigen values? $$\hat{H}\left|\varphi_i\right\rangle = E_i\left|\varphi_i\right\rangle$$

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

represented in certain basis

Look up linear algebra:

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

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

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

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

Degenerate (ontaarde) states

What if $V_1 = V_2 = V_o$?

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

$$E_1 = V_0, \quad E_2 = V_0, \quad E_3 = V_3$$

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

$$\begin{cases} \hat{H}\left|\varphi_1\right\rangle = V_o\left|\varphi_1\right\rangle \\ \hat{H}\left|\varphi_2\right\rangle = V_o\left|\varphi_2\right\rangle \\ \hat{H}\left|\varphi_3\right\rangle = V_3\left|\varphi_3\right\rangle \end{cases}$$

Degenerate (ontaarde) states

$$\begin{cases} \hat{H}|\varphi_1\rangle = V_o|\varphi_1\rangle \\ \hat{H}|\varphi_2\rangle = V_o|\varphi_2\rangle \\ \hat{H}|\varphi_3\rangle = V_3|\varphi_3\rangle \end{cases}$$

$$\hat{H}\left(\alpha|\varphi_1\rangle + \beta|\varphi_2\rangle\right) = V_o\left(\alpha|\varphi_1\rangle + \beta|\varphi_2\rangle\right)$$

$$\left[\hat{H}, \hat{B}\right] = 0$$

$$\hat{B}\left(\hat{H}|\varphi_1\rangle\right) = \hat{B}V_o|\varphi_1\rangle = V_o\hat{B}|\varphi_1\rangle = \hat{H}\left(\hat{B}|\varphi_1\rangle\right)$$

but also $\hat{B}|\varphi_1\rangle = \gamma\left(\alpha|\varphi_1\rangle + \beta|\varphi_2\rangle\right)$

$|\varphi_1\rangle$ **not an eigen state of** $\hat{B}$ **!**

(see book p. 137)

Degenerate (ontaarde) states

$$\left[\hat{H}, \hat{B}\right] = 0$$

$$\hat{B}\left(\hat{H}|\varphi_1\rangle\right) = \hat{B}V_o|\varphi_1\rangle = V_o\hat{B}|\varphi_1\rangle = \hat{H}\left(\hat{B}|\varphi_1\rangle\right)$$

but also $\hat{B}|\varphi_1\rangle = \gamma\left(\alpha|\varphi_1\rangle + \beta|\varphi_2\rangle\right)$

$|\varphi_1\rangle$ **not an eigen state of** $\hat{B}$ **!**

More clear for $\hat{H} = \dfrac{\hat{p}^2}{2m} = \dfrac{\hbar^2\hat{k}^2}{2m}$

$$\hat{B} = \hat{p} = \hbar\hat{k}$$

Degenerate (ontaarde) states

Conclusie:

Als 2 operatoren commuteren ($\left[\hat{H},\hat{B}\right]=0$), en er is GEEN ontaarding

dan hebben ze dezelfde eigenvectoren (eigenfuncties).

Als 2 operatoren commuteren ($\left[\hat{H},\hat{B}\right]=0$), en er WEL ontaarding

dan hebben ze mogelijke verschillende eigenvectoren (eigenfuncties).

Time-evolution operator $\hat{U}$

For system with time-independent Hamiltonian $\hat{H}_0$

$$\left|\Psi(t)\right\rangle=\hat{U}\left|\Psi(t_0)\right\rangle=e^{\frac{-i\hat{H}_0(t-t_0)}{\hbar}}\left|\Psi(t_0)\right\rangle$$

$$\left\langle\Psi(t)\right|=\left\langle\Psi(t_0)\right|\hat{U}^+=\left\langle\Psi(t_0)\right|e^{\frac{+i\hat{H}_0(t-t_0)}{\hbar}}$$

How does some physical property A depend on time?

$$\left\langle\hat{A}\right\rangle(t)=\left\langle\Psi(t)\right|\hat{A}\left|\Psi(t)\right\rangle$$

$$=\left\langle\Psi(t_0)\right|\hat{U}^+\ \hat{A}\ \hat{U}\left|\Psi(t_0)\right\rangle$$

$$=\left\langle\Psi(t_0)\right|e^{\frac{+i\hat{H}_0(t-t_0)}{\hbar}}\ \hat{A}\ e^{\frac{-i\hat{H}_0(t-t_0)}{\hbar}}\left|\Psi(t_0)\right\rangle$$

Voorruitblik:

Schrödinger (nu) versus Heisenberg picture

How does some physical property A depend on time?

$$\left\langle \hat{A} \right\rangle(t) = \left\langle \Psi(t) \right| \hat{A} \left| \Psi(t) \right\rangle$$

$$= \left\langle \Psi(t_0) \right| \hat{U}^+ \ \hat{A}\ \hat{U} \left| \Psi(t_0) \right\rangle$$

$$= \underbrace{\left\langle \Psi(t_0) \right| e^{\frac{+i\hat{H}_0(t-t_0)}{\hbar}}}\ \hat{A}\ \underbrace{e^{\frac{-i\hat{H}_0(t-t_0)}{\hbar}} \left| \Psi(t_0) \right\rangle}$$

Schrödinger: Tijdsafhankelijke toestanden

$$\left\langle \hat{A} \right\rangle(t) = \left\langle \Psi(t_0) \right| \underbrace{e^{\frac{+i\hat{H}_0(t-t_0)}{\hbar}}\ \hat{A}\ e^{\frac{-i\hat{H}_0(t-t_0)}{\hbar}}} \left| \Psi(t_0) \right\rangle$$

Heisenberg: Tijdsafhankelijke observabelen

Time-evolution operator $\hat{U}$

For system with time-independent Hamiltonian $\hat{H}_0$

Say it starts in a state $\left| \Psi(t=0) \right\rangle = \alpha \left| \varphi_1 \right\rangle + \beta \left| \varphi_2 \right\rangle$ (energy eigenvectors)

How does some physical property A depend on time?

$$\left\langle \hat{A} \right\rangle(t) = \left\langle \Psi(t) \right| \hat{A} \left| \Psi(t) \right\rangle$$

$$= \left\langle \Psi(0) \right| \hat{U}^+ \ \hat{A}\ \hat{U} \left| \Psi(0) \right\rangle$$

$$= \left\langle \Psi(0) \right| e^{\frac{+i\hat{H}_0 t}{\hbar}}\ \hat{A}\ e^{\frac{-i\hat{H}_0 t}{\hbar}} \left| \Psi(0) \right\rangle$$

$$= \left[\alpha^* e^{\frac{+iE_1 t}{\hbar}} \left\langle \varphi_1 \right| + \beta^* e^{\frac{+iE_2 t}{\hbar}} \left\langle \varphi_2 \right| \right] \hat{A} \left[\alpha\, e^{\frac{-iE_1 t}{\hbar}} \left| \varphi_1 \right\rangle + \beta\, e^{\frac{-iE_2 t}{\hbar}} \left| \varphi_2 \right\rangle \right]$$

$$= \alpha^* \alpha \left\langle \varphi_1 \right| \hat{A} \left| \varphi_1 \right\rangle + \beta^* \beta \left\langle \varphi_2 \right| \hat{A} \left| \varphi_2 \right\rangle + \alpha^* \beta\, e^{\frac{+i(E_1-E_2)t}{\hbar}} \left\langle \varphi_1 \right| \hat{A} \left| \varphi_2 \right\rangle + \alpha \beta^* e^{\frac{+i(E_2-E_1)t}{\hbar}} \left\langle \varphi_1 \right| \hat{A} \left| \varphi_2 \right\rangle^*$$

$$= \alpha^* \alpha \left\langle \varphi_1 \right| \hat{A} \left| \varphi_1 \right\rangle + \beta^* \beta \left\langle \varphi_2 \right| \hat{A} \left| \varphi_2 \right\rangle + 2\,\mathbf{Re}\left(\alpha^* \beta\, e^{\frac{+i(E_1-E_2)t}{\hbar}} \left\langle \varphi_1 \right| \hat{A} \left| \varphi_2 \right\rangle \right)$$

Last term in general cosine with amplitude <u>and phase</u>

Free particle - Gaussian wave packet

x-representation and k-representation

$$\Psi(x) \quad \overset{\mathbf{F}}{\leftrightarrow} \quad \overline{\Psi}(k)$$

$$\Psi(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \overline{\Psi}(k) e^{ikx}\, dk$$

$$\overline{\Psi}(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \Psi(x) e^{-ikx}\, dx$$

Fourier transforms in book

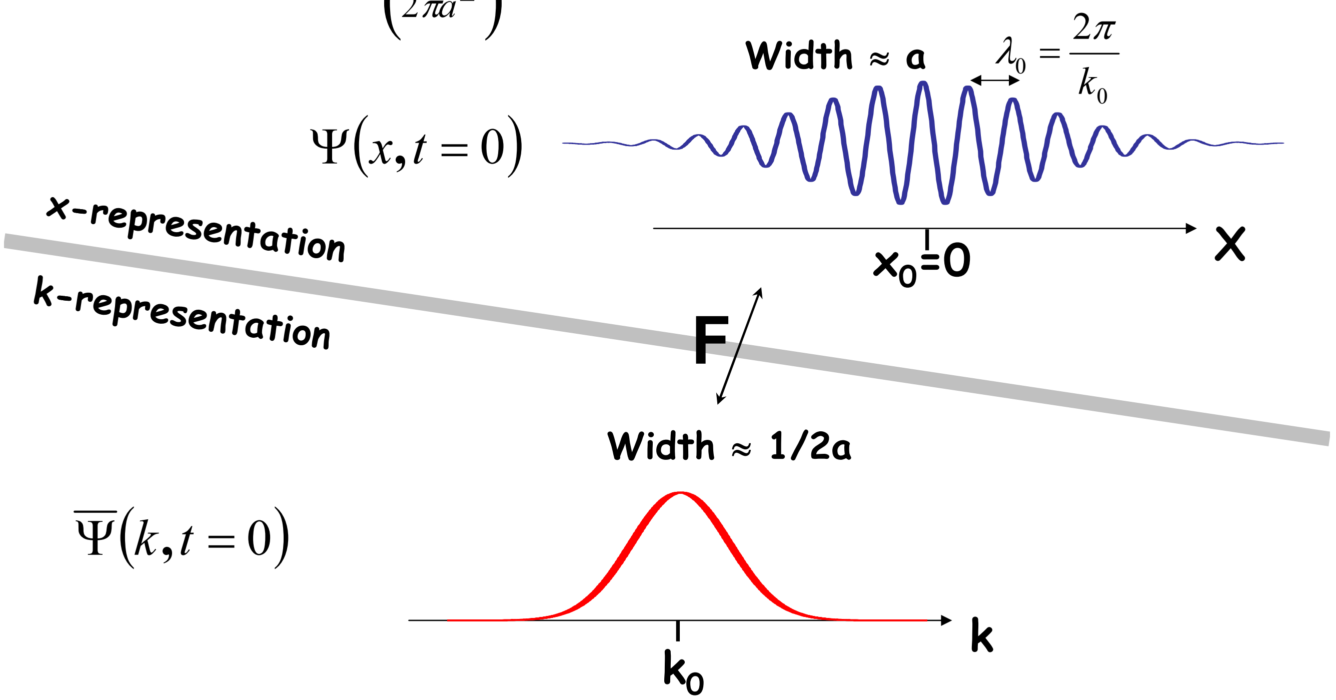
between x-representation and k-representation (or n-representation)

⇒ A different way to represent the *same* state

p. 100 and 117	expansion into a series of discrete states
p. 102	projection onto k-states (plane waves)
p. 125	delta function in x-representation
p. 122 and 158	square wave in x-representation
p. 156	Wave packet in x- and p-representation
p. 160	Gaussian in x- and p-representation
p. 849 and 857	Appendix A, C

Dit overzichtje met nog wat uitleg zit ook in "StofOverzicht – Concepten" op het web

$$\Psi(x,t=0)=\frac{1}{\left(2\pi a^2\right)^{1/4}}e^{ik_0x}e^{-x^2/4a^2}$$

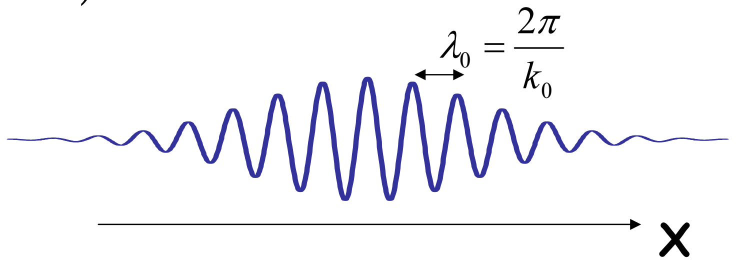


$$\overline{\Psi}(k,t=0)=\left(\frac{4a^2}{2\pi}\right)^{1/4}e^{-a^2(k-k_0)^2}$$

(see book p. 160)

$$\Psi(x,t=0)=\frac{1}{\left(2\pi a^2\right)^{1/4}}e^{ik_0x}e^{-x^2/4a^2}$$

$$\hat{H}=\frac{(\hbar\hat{k})^2}{2m}$$



Time-evolution:

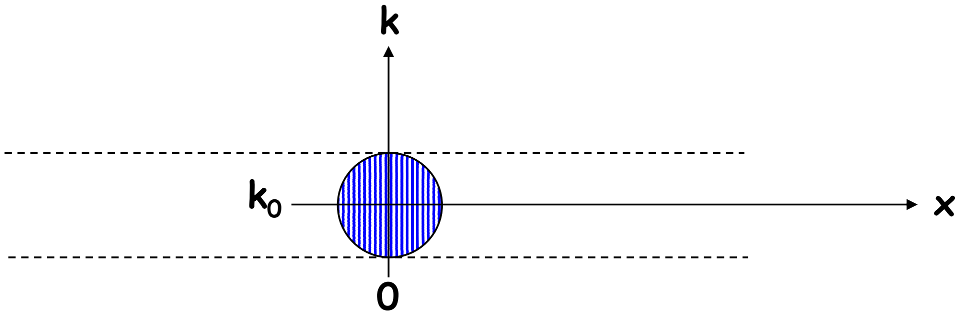
$$\Psi(x,t)=\hat{U}\,\Psi(x,t=0)$$

$$=e^{\frac{-i\hat{H}t}{\hbar}}\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\overline{\Psi}(k)e^{ikx}\,dk$$

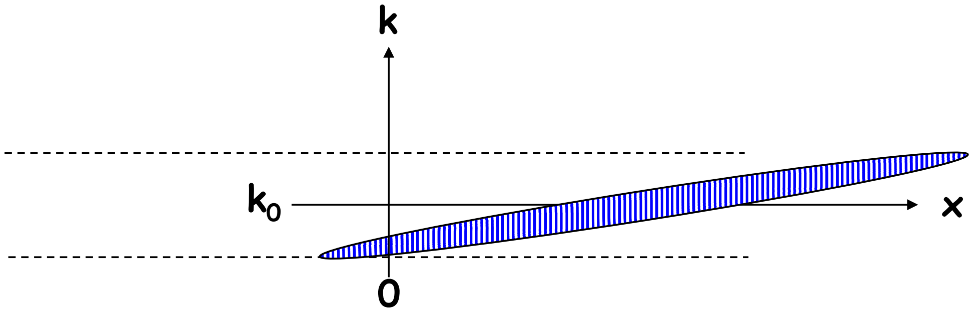
Easier to evaluate with Fourier transform!

$$=\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\overline{\Psi}(k)e^{i(kx-\omega t)}\,dk$$

$t = 0$



$t > 0$



We use here that one can represent a state also in the x-k plane

Using the commutator bracket to describe time evolution

$$\frac{d\langle \hat{A} \rangle}{dt} = \frac{\partial \langle \hat{A} \rangle}{\partial t} = \frac{\partial \langle \Psi | \hat{A} | \Psi \rangle}{\partial t}$$

$$= \frac{\partial \langle \Psi |}{\partial t} \hat{A} | \Psi \rangle + \langle \Psi | \hat{A} \frac{\partial | \Psi \rangle}{\partial t} + \langle \Psi | \frac{\partial \hat{A}}{\partial t} | \Psi \rangle$$

$$\frac{\partial \langle \Psi |}{\partial t} = \langle \Psi | \frac{i\hat{H}^{+}}{\hbar}$$

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

$$\frac{\partial \langle \hat{A} \rangle}{\partial t} = \frac{i}{\hbar} \left(\langle \Psi | \hat{H}^{+} \hat{A} | \Psi \rangle - \langle \Psi | \hat{A} \hat{H} | \Psi \rangle \right) + \langle \Psi | \frac{\partial \hat{A}}{\partial t} | \Psi \rangle$$

$$\hat{H} = \hat{H}^{+}$$

$$\frac{d\langle \hat{A} \rangle}{dt} = \langle \Psi | \frac{i}{\hbar} \left[\hat{H}, \hat{A} \right] + \frac{\partial \hat{A}}{\partial t} | \Psi \rangle$$

$$\boxed{\frac{d\langle \hat{A} \rangle}{dt} = \frac{i}{\hbar} \langle \Psi | \left[\hat{H}, \hat{A} \right] | \Psi \rangle}$$

Will be generalized later

Voorbeeldje, laat zien dat voor deeltje met $\hat{H} = \frac{\hat{p}^2}{2m} + \hat{V}$, $\hat{V} = V(x)$

$$\frac{d\langle \hat{x} \rangle}{dt} = \left\langle \frac{\hat{p}}{m} \right\rangle \qquad \frac{d\langle \hat{p} \rangle}{dt} = -\left\langle \frac{\partial \hat{V}}{\partial \hat{x}} \right\rangle$$

$$\left[\hat{p}, \hat{x}^2\right] = \left[\hat{p}, \hat{x}\right]\hat{x} + \hat{x}\left[\hat{p}, \hat{x}\right] = -2i\hbar\hat{x}$$
$$\left[\hat{p}, \hat{x}^3\right] = \left[\hat{p}, \hat{x}\right]\hat{x}^2 + \hat{x}\left[\hat{p}, \hat{x}^2\right] = -3i\hbar\hat{x}^2$$

Use: $\left[\hat{p}, \hat{x}^n\right] = -i\hbar n\hat{x}^{n-1}$

$$\left[\hat{p}, \hat{x}^{n+1}\right] = \left[\hat{p}, \hat{x}\hat{x}^n\right] = \left[\hat{p}, \hat{x}\right]\hat{x}^n + \hat{x}\left[\hat{p}, \hat{x}^n\right] = -i\hbar\hat{x}^n - i\hbar\hat{x}n\hat{x}^{n-1} = -i\hbar(n+1)\hat{x}^n$$

$$\left[\hat{p}, G(\hat{x})\right] = -i\hbar\frac{\partial G(\hat{x})}{\partial \hat{x}}$$

Constant of motion: $\hat{H}$ and $\hat{A}$ commute

$$\left[\hat{H}, \hat{A}\right] = 0 \qquad \Rightarrow$$

$$\frac{d\langle \hat{A} \rangle}{dt} = \frac{i}{\hbar}\langle \Psi | \left[\hat{H}, \hat{A}\right] | \Psi \rangle = 0$$

Already known from time-evolution operator $\hat{U}$

For system with time-independent Hamiltonian $\hat{H}_0$

Say it starts in a state $|\Psi(t=0)\rangle = \alpha|\varphi_1\rangle + \beta|\varphi_2\rangle$ (energy eigenvectors)

How does some physical property A depend on time?

$$\langle \hat{A} \rangle(t) = \langle \Psi(t)|\, \hat{A}\, |\Psi(t)\rangle$$
$$= \langle \Psi(0)|\, \hat{U}^{+}\, \hat{A}\, \hat{U}\, |\Psi(0)\rangle$$
$$= \langle \Psi(0)|\, e^{\frac{+i\hat{H}_0 t}{\hbar}}\, \hat{A}\, e^{\frac{-i\hat{H}_0 t}{\hbar}}\, |\Psi(0)\rangle$$
$$= \left[\alpha^* e^{\frac{+iE_1 t}{\hbar}} \langle \varphi_1| + \beta^* e^{\frac{+iE_2 t}{\hbar}} \langle \varphi_2| \right] \hat{A} \left[\alpha\, e^{\frac{-iE_1 t}{\hbar}} |\varphi_1\rangle + \beta\, e^{\frac{-iE_2 t}{\hbar}} |\varphi_2\rangle \right]$$
$$= \alpha^* \alpha \langle \varphi_1|\hat{A}|\varphi_1\rangle + \beta^* \beta \langle \varphi_2|\hat{A}|\varphi_2\rangle + 2\,\mathbf{Re}\left(\alpha^* \beta\, e^{\frac{+i(E_1 - E_2)t}{\hbar}} \langle \varphi_1|\hat{A}|\varphi_2\rangle \right)$$

Ehrenfest's principle

Equations of motion for expectation values correspond to classical equations.

Only works out for linear systems! (energy $\propto$ x^2 and p^2) – See problem 6.25

$$\frac{d\langle \hat{x} \rangle}{dt} = \left\langle \frac{\hat{p}}{m} \right\rangle \qquad \frac{d\langle \hat{p} \rangle}{dt} = -\left\langle \frac{\partial \hat{V}}{\partial \hat{x}} \right\rangle$$

Samenvatting:

1. Meer over tijdsevolutie
2. Degenaracy

Volgende college:

C.S.C.O – Hilbert space basis
Conservation laws
Parity
Example about different representations