Kwantumfysica I

2008-2009

Hoorcollege vrijdag 12 december 2008

Vragen n.a.v. stof tot nu toe?

Vandaag:

Example about different representations,
Fourier transfrom, decomposition

C.S.C.O. - States of systems with more D.O.F.

Conservation laws

Parity

Example representations, Fourier

The <u>same</u> *state* of a quantum system can be *represented* in many different ways.

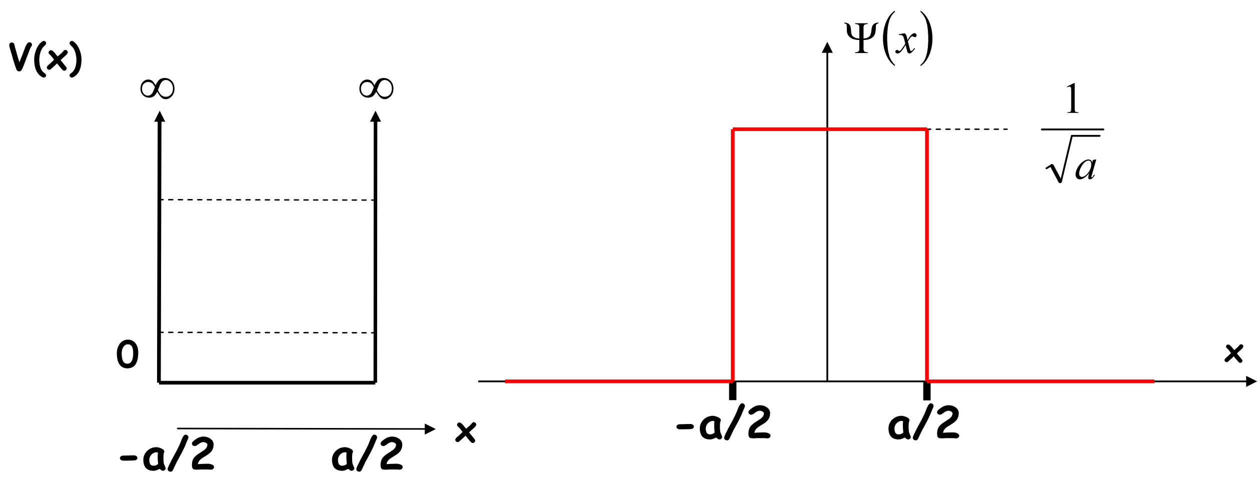
-a wavefunction that is a function of position *x*

-a wavefunction that is a function of wave number *k* (or, $p_x = \hbar k$)

-a superposition of energy eigenstates

-x-or p-representation versus Dirac notation

-more………

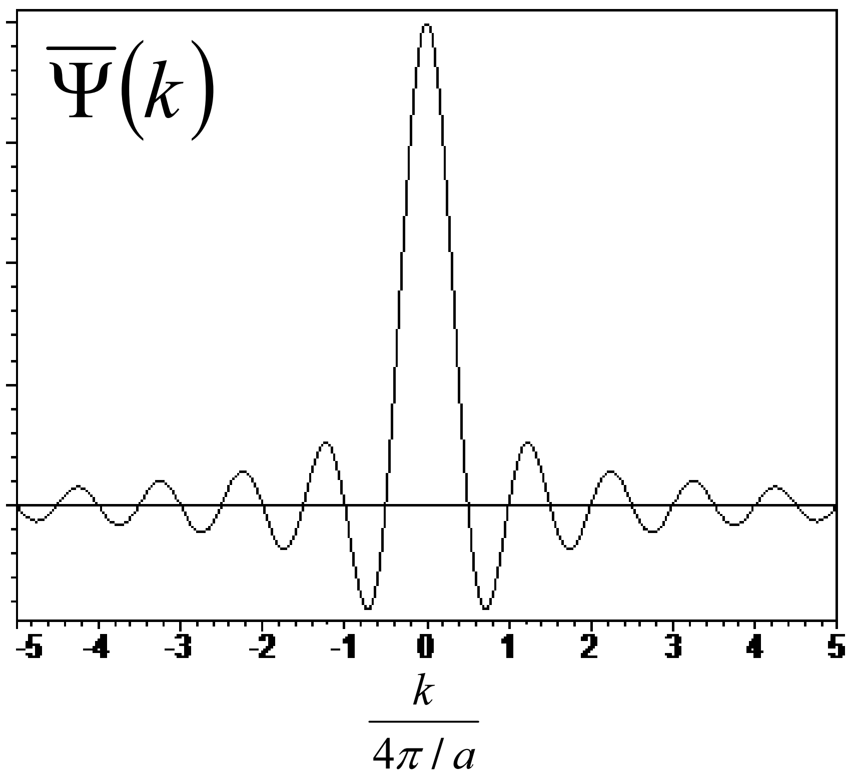


$$\Psi(x) \quad \leftrightarrow \quad \overline{\Psi}(k)$$

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

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

$$\overline{\Psi}(k) = \frac{\sqrt{a}}{\sqrt{2\pi}} \frac{\sin\left(\frac{a}{2} k\right)}{\frac{a}{2} k}$$



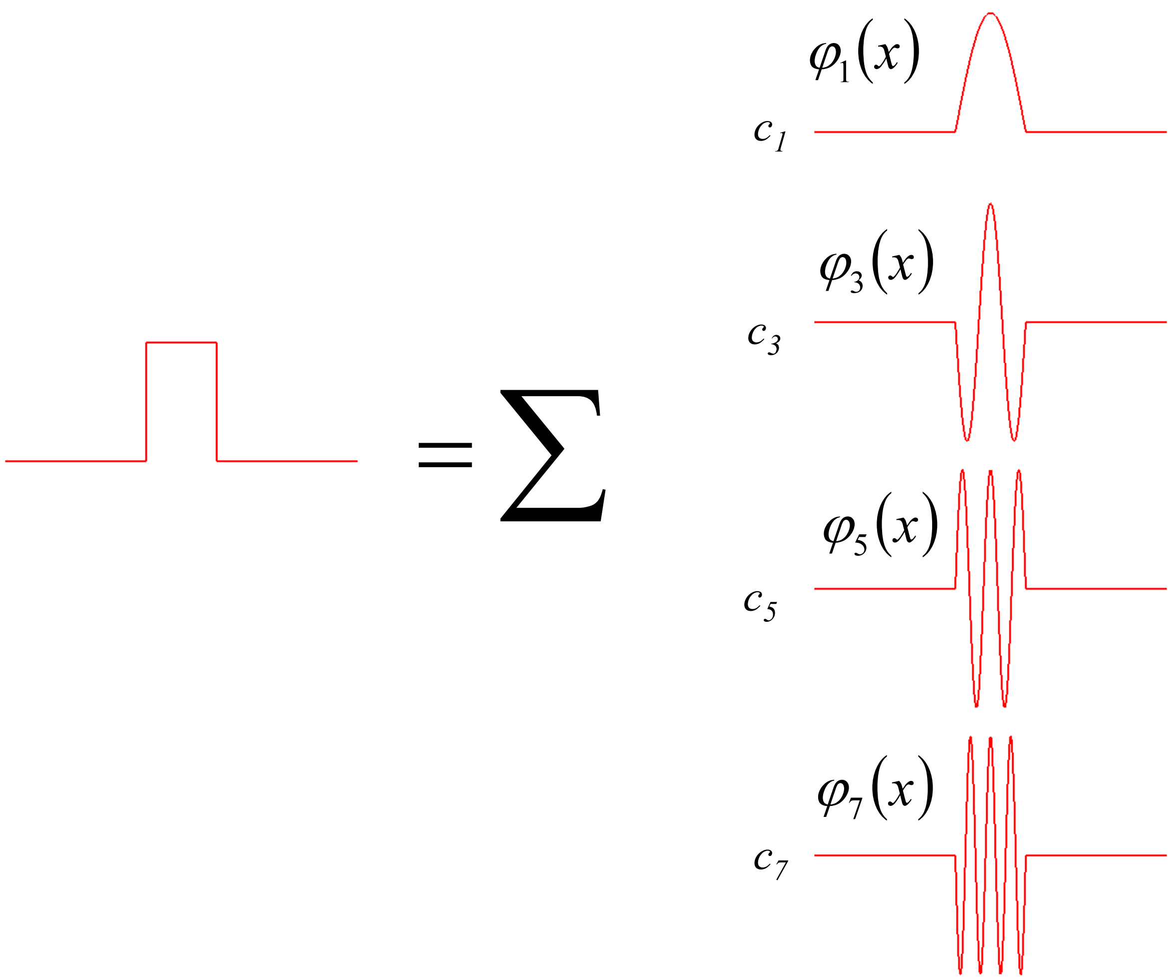
$$\left|\Psi\right\rangle = \sum_n c_n \left|\varphi_n\right\rangle$$

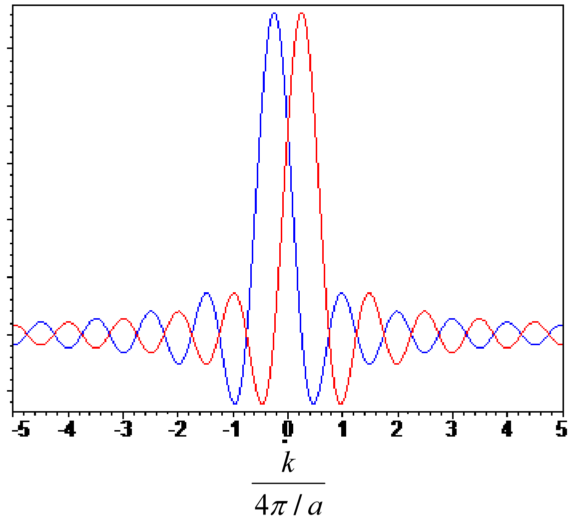
What are the $\left|\varphi_n\right\rangle$ **?**

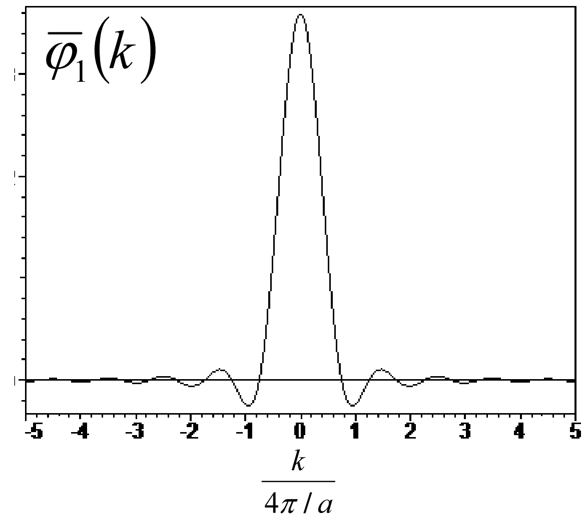
What are the c_n **?**

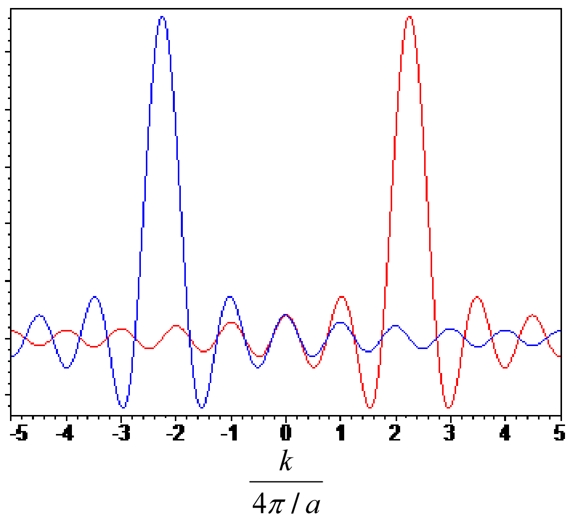
$$\begin{cases} \varphi_n(x) = \sqrt{\tfrac{2}{a}}\,\mathbf{sin}\left(\tfrac{n\pi x}{a}\right), & n \text{ even} \\ \varphi_n(x) = \sqrt{\tfrac{2}{a}}\,\mathbf{cos}\left(\tfrac{n\pi x}{a}\right) & n \text{ odd} \end{cases}$$

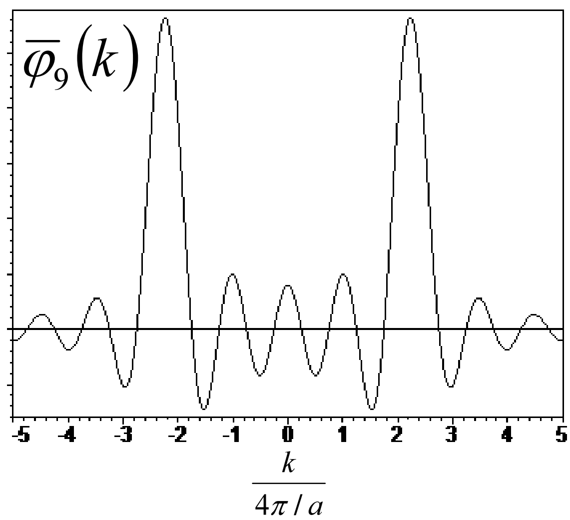
$$c_n = \left\langle \varphi_n \middle| \Psi \right\rangle$$

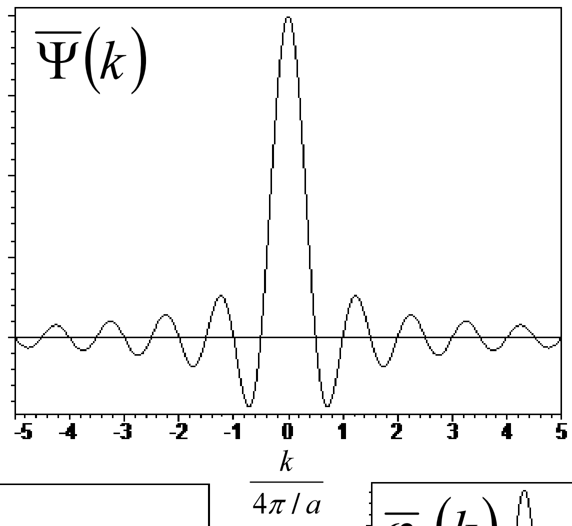


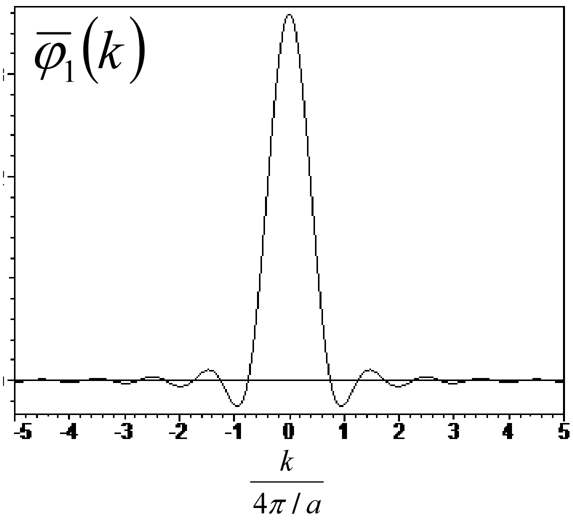

-5 -4 -3 -2 -1 0 1 2 3 4 5
$\frac{k}{4\pi/a}$

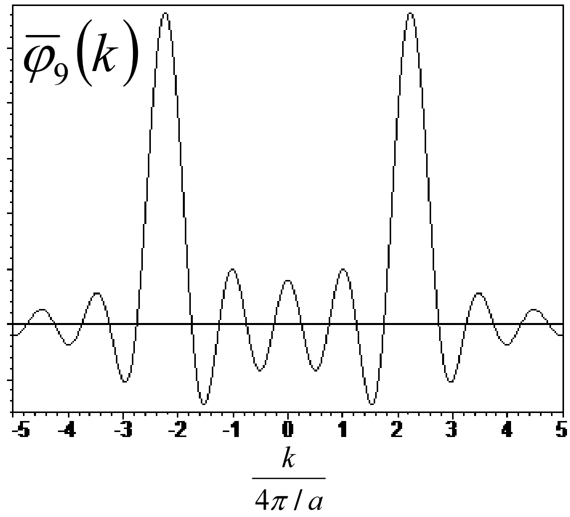

$\overline{\varphi}_1(k)$
-5 -4 -3 -2 -1 0 1 2 3 4 5
$\frac{k}{4\pi/a}$

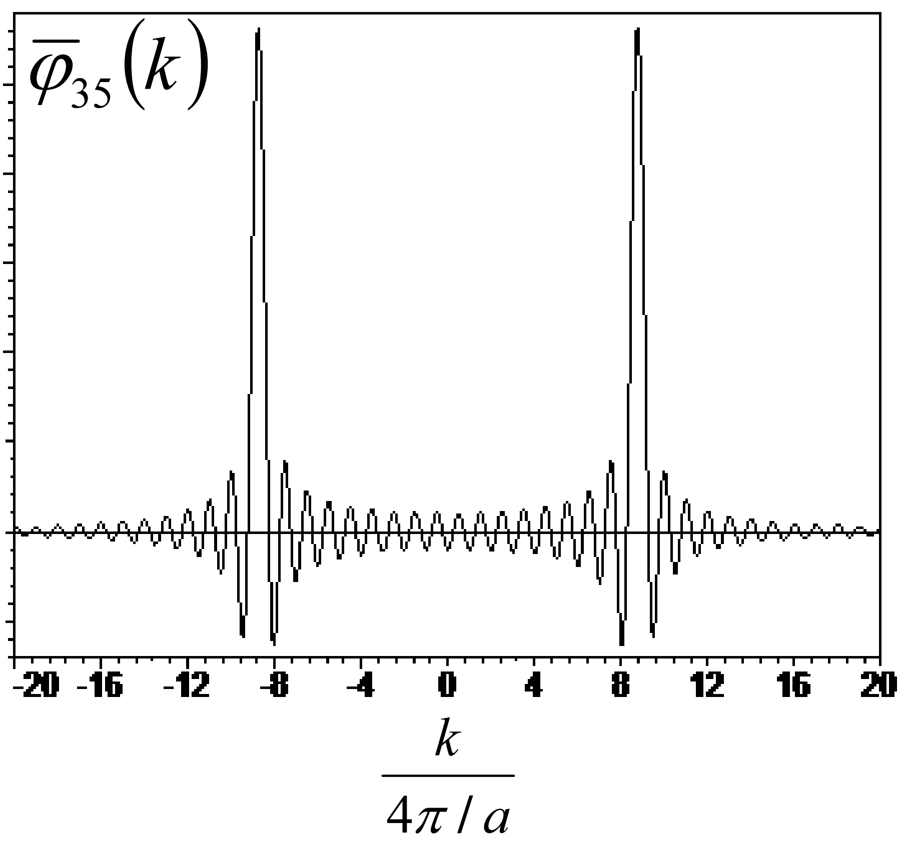

-5 -4 -3 -2 -1 0 1 2 3 4 5
$\frac{k}{4\pi/a}$


$\overline{\varphi}_9(k)$
-5 -4 -3 -2 -1 0 1 2 3 4 5
$\frac{k}{4\pi/a}$


$\overline{\Psi}(k)$
-5 -4 -3 -2 -1 0 1 2 3 4 5
$\frac{k}{4\pi/a}$


$\overline{\varphi}_1(k)$
-5 -4 -3 -2 -1 0 1 2 3 4 5
$\frac{k}{4\pi/a}$


$\overline{\varphi}_9(k)$
-5 -4 -3 -2 -1 0 1 2 3 4 5
$\frac{k}{4\pi/a}$


$\overline{\varphi}_{35}(k)$
-20 -16 -12 -8 -4 0 4 8 12 16 20
$\frac{k}{4\pi/a}$

Verder:

C.S.C.O. - States of systems with more D.O.F.

Conservation laws

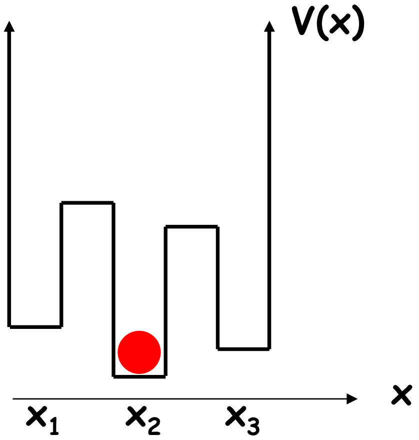
Parity

C.S.C.O.

(book p. 143 – 145)

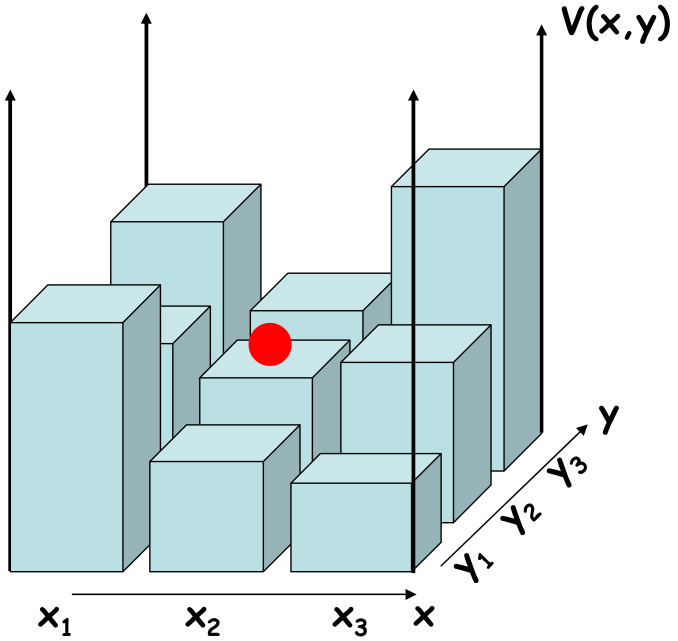
1D systeem

Mechanisch systeem, met 3 toestanden



2D systeem

Mechanisch systeem, met 3 toestanden in x en y richting



What are the commutation relations for $\hat{x}, \hat{p}_x, \hat{y}, \hat{p}_y$

$$[\hat{x}, \hat{p}_x] = i\hbar$$
$$[\hat{y}, \hat{p}_y] = i\hbar$$
$$[\hat{x}, \hat{y}] = 0$$
$$[\hat{p}_x, \hat{p}_y] = 0$$
and $[\hat{x}, \hat{x}] = 0$ etc.

C.S.C.O

Complete set of **commuting** observables

A minimal set of observables whose eigenvectors can represent all possible states of the system $\Rightarrow$ **Hilbert space**

Not a unique set, but a minimal set

Confusing (a bit wrong) in the book on p. 144

Better example, 2D case on previous slide.

A C.S.C.O. is $\{\hat{x}, \hat{y}\}$

or $\{\hat{p}_x, \hat{p}_y\}$

or $\{\hat{x}, \hat{p}_y\}$

but NOT $\{\hat{x}, \hat{p}_y^2\}$

and NOT $\{\hat{x}, \hat{p}_x \hat{p}_y\}$

$$\hat{H} = \frac{\hat{p}^2}{2m} = \frac{\hbar^2 \hat{k}^2}{2m}$$
$$\hat{p} = \hbar \hat{k}$$
$$[\hat{H}, \hat{p}] = 0$$

Approach in book relevant later for 3D atoms, not for 1D case.

Let us take for the 2D case the C.S.C.O.

C.S.C.O. = $\{\hat{x}, \hat{y}\}$

<u>Orthonormal</u> basis vectors $|x\rangle \otimes |y\rangle = |x\rangle |y\rangle = |x, y\rangle$

$$|\Psi\rangle = \iint c_{xy} |x, y\rangle dx\, dy$$

This is a good C.S.C.O. and the above wavefunction has information about EVERYTHING there is to know about the system.

Conservation laws (previous lecture)

for isolated systems with constant Hamiltonian

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

$\hat{H}$ and $\hat{A}$ commute: $[\hat{H}, \hat{A}] = 0 \qquad \Rightarrow$

Everye operator that commutes with the Hamiltonian, describes a property of the system that is <u>conserved</u>.

$\Rightarrow$ Constants of motion
Invariance

Besides <u>constants of motion</u> (earlier in lecture):

Invariance or conservation of other properties (all these properties can be described by an operator)

-symmetry and parity
(parity operator)

-invariance of laws when changing reference frame
(translation and rotation operators)

Conservation of parity - parity operator

Odd parity $f(-x) = -f(x)$

Even parity $f(-x) = +f(x)$

Effect of parity operator on a function:

$$\hat{\mathbf{P}}\, f(x) = f(-x)$$

Eigenstates of the parity operator:

$$\hat{\mathbf{P}}\, g(x) = \alpha\, g(x)$$

$$\Rightarrow \begin{cases} \alpha = +1 \;, & \text{all even } g(x) \\ \alpha = -1 \;, & \text{all odd } g(x) \end{cases}$$

Note: every function can be written as a sum of an even and an odd function

book p. 177

$$\hat{H} = \frac{\hat{p}^2}{2m} + \hat{V}, \qquad \hat{V} = V(x), \quad \text{is symmetric(even) in } x$$

$$\hat{\mathbf{P}}\,\hat{V}(x)\Psi(x) = \hat{V}(-x)\Psi(-x) = \hat{V}(x)\hat{\mathbf{P}}\,\Psi(x)$$

$$\Rightarrow \hat{\mathbf{P}}\,\hat{V} = \hat{V}\,\hat{\mathbf{P}}$$

$$\Rightarrow \left[\hat{V}, \hat{\mathbf{P}}\right] = 0$$

Also $\left[\hat{p}_x^2, \hat{\mathbf{P}}\right] = 0$ **(See problem 6.16)** $\hat{p}_x$ is odd $\Rightarrow \hat{p}_x^2$ is even

$\Rightarrow \left[\hat{H}, \hat{\mathbf{P}}\right] = 0 \Rightarrow$ **As a function of time, the parity (symmetry) of the wavefunction is constant.**

$\Rightarrow$ **Strong influence on dynamics of systems: Determines <u>selection rules</u>, decay rates, …..**

Strong influence on dynamics of systems:
Determines selection rules, decay rates, ….. (not yet in chapter 6)

$$\hat{\mathrm{P}} = \hat{\mathrm{P}}^{-1}$$

$$\begin{cases} \hat{\mathrm{P}}\,\hat{A}_{even}\,\hat{\mathrm{P}} = +\hat{A}_{even}, & \text{even operator} \\ \hat{\mathrm{P}}\,\hat{A}_{odd}\,\hat{\mathrm{P}} = -\hat{A}_{odd}, & \text{odd operator} \end{cases}$$

Say $\hat{A}_{even}$ is an even operator, say $\left|\varphi_{even}\right\rangle \leftrightarrow \varphi_{even}(x)$ even

$\hat{\mathrm{P}} = \hat{\mathrm{P}}^{-1}$ $\qquad \left|\varphi_{odd}\right\rangle \leftrightarrow \varphi_{odd}(x)$ odd

$$\left\langle \varphi_{even} \right| \hat{A}_{even} \left| \varphi_{odd} \right\rangle =$$

$$\int \varphi_{even}(x)\hat{\mathrm{P}}\,\hat{A}_{even}\,\hat{\mathrm{P}}\,\varphi_{odd}(x)\,dx =$$

$$\int \varphi_{even}(-x)\hat{A}_{even}\varphi_{odd}(-x)\,dx =$$

$$\int \left(+\varphi_{even}(x)\right)\hat{A}_{even}\left(-\varphi_{odd}(x)\right)dx =$$

$$-\left\langle \varphi_{even} \right| \hat{A}_{even} \left| \varphi_{odd} \right\rangle = 0 \quad \text{, since equal to starting arguement}$$

Cohen T. book p. 192

Samenvatting:

Example about different representations,
Fourier transfrom, decomposition

C.S.C.O. - States of systems with more D.O.F.
$\Rightarrow$ Hilbert space basis

Conservation laws

Parity

Volgende week: H7

Harmonic oscillator
Tunnel effect
Scattering