1/8

Uitwerking Final Exam Kwantumfysica 1

26 juni 2006

Problem 1

a) The two quantum point particles can each move in 3 spatial dimensions $\Rightarrow$ 6 degrees of freedom

<u>Note</u> 1) We assume here point particles. If it are not point particles, each particle has also 3 rotational degrees of freedom. More complex particles, like atoms, also have internal degrees of freedom.

2) For particle 1 in x-direction, there is the operator $\hat{x}_1$ for position, and $\hat{p}_{x1}$ for momentum, but it is only 1 degree of freedom! Not 2!

b) Pairs that do <u>not</u> commute:

$$\left\{\begin{array}{l} [\hat{x}_1, \hat{p}_{x1}] = i\hbar \\ [\hat{y}_1, \hat{p}_{y1}] = i\hbar \\ [\hat{z}_1, \hat{p}_{z1}] = i\hbar \\ [\hat{x}_2, \hat{p}_{x2}] = i\hbar \\ [\hat{y}_2, \hat{p}_{y2}] = i\hbar \\ [\hat{z}_2, \hat{p}_{z2}] = i\hbar \end{array}\right.$$

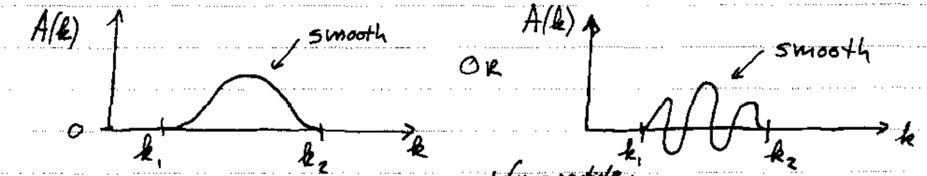
All other paired combinations of the 12 mentioned operators do commute, and have therefore for example $[\hat{x}_1, \hat{p}_{y1}] = 0$, $[\hat{x}_1, \hat{z}_1] = 0$ and $[\hat{x}_1, \hat{x}_2] = 0$.

This can be understood by considering that any observable of particle 1, and any observable of particle 2 can be measured simultaneously with unlimited accuracy. The same holds for observables of the same particle but for a different spatial direction.

2/8

Problem 2

a) The state is a superposition of plane waves $e^{i(kx-\omega t)}$, each with a particular amplitude $A(k)$. The superposition only contains plane waves with a wave number k in the range $k_1 < k < k_2$, as for example



It represents a wave packet (for a particle) with a momentum of about $\langle p_x \rangle \approx \frac{\hbar k_1 + \hbar k_2}{2}$, and a quantum uncertainty in momentum $\Delta p_x \approx \hbar \Delta k \approx \hbar \frac{k_2 - k_1}{2}$.

b) The phase velocity is the propagation speed of each argument with a constant phase $(kx-\omega t)$ for each plane wave (with its particular k) $\Rightarrow$

$kx - \omega t$ is constant $\Rightarrow \frac{dx}{dt} = V_{phase} = \frac{\omega}{k}$ (is >0)

c) Here we consider a mechanical, massive free particle. The Hamiltonian is therefore

$\hat{H} = \frac{\hat{p}_x^2}{2m} = \frac{\hbar \hat{k}^2}{2m} \Rightarrow$ the energy is $\frac{\hbar k^2}{2m}$ for a plane wave with wave number k, and the time evolution of such a plane wave is from a factor $e^{-i\hat{H}t/\hbar} \Rightarrow$ Gives $e^{-\frac{i}{\hbar}\frac{\hbar k^2}{2m}t}$ for a plane wave with certain k.

3/8

This can be used to define

$$\hbar\omega = \frac{\hbar^2 k^2}{2m} \Rightarrow \omega = \frac{\hbar k^2}{2m}$$

(the so-called dispersion relation)

d) The group velocity is $V_{group} = \frac{\partial \omega}{\partial k} \Rightarrow$

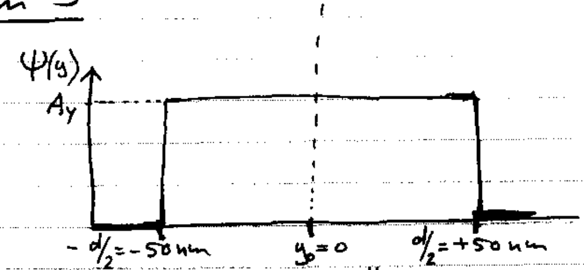
$V_{group} = 2\frac{\hbar k}{2m}$. This should be evaluated for the k-values that are typical (most present) in the wave packet described by $A(k)$ $\Rightarrow$

For this state $V_{group} \approx \frac{\hbar\left(\frac{k_1+k_2}{2}\right)}{m} \approx \frac{\langle P_x \rangle}{m}$

It is the propagation speed of the wave packet

Problem 3

a)



$$\int_{-\infty}^{\infty} |\Psi(y)|^2 dy = 1 \Rightarrow \int_{-d/2}^{d/2} A_y^2\, dy = 1 \Rightarrow A_y^2 \cdot d = 1$$

$$\Rightarrow A_y = \sqrt{\frac{1}{d}} = \sqrt{\frac{1}{100\,nm}} \approx 3.16 \cdot 10^3\ m^{-1/2}$$

b)

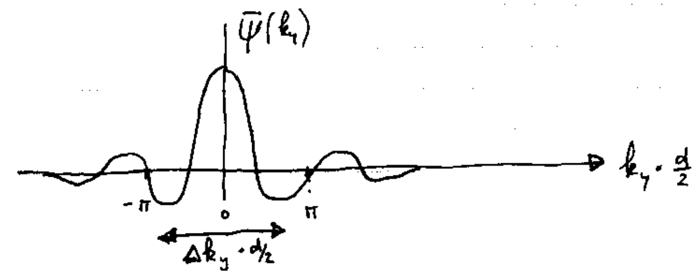
$$\bar{\Psi}(k_y) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \Psi(y)\, e^{-ik_y y} dy$$

$$= \frac{1}{\sqrt{2\pi}} \int_{-d/2}^{d/2} A_y e^{-ik_y y} dy = \frac{1}{ik_y\sqrt{2\pi}} \left[A_y e^{-ik_y y}\right]_{-d/2}^{d/2}$$

$$= \frac{2A_y}{\sqrt{2\pi}} \frac{\sin\left(\frac{d}{2}k_y\right)}{k_y} = \frac{dA_y}{\sqrt{2\pi}} \frac{\sin\left(\frac{d}{2}k_y\right)}{\frac{d}{2}k_y}$$

c) The answer on b) is a sinc function, which is centered around $k_y = 0$, and which decreases in amplitude over a range

$$\frac{1}{2}\Delta k_y \approx \frac{2\pi}{d} \Rightarrow \Delta k_y \approx \frac{2\pi}{d} \Rightarrow \Delta p_y \approx \frac{2\pi\hbar}{d} \approx \frac{h}{d}$$



d) After the screen, the electron is a free particle. For a free particle, the momentum properties do not change in time $\Rightarrow$ Δp_y stays constant with time.

Note: this can for example be seen from:

Hamiltonian for the dynamics in y-direction is

$$\hat{H}_y = \frac{\hat{p}_y^2}{2m}$$

$$\Delta p_y = \sqrt{\langle \hat{p}_y^2 \rangle - \langle \hat{p}_y \rangle^2}$$, so we should look at

$$\frac{d\langle \hat{p}_y \rangle}{dt} = \frac{i}{\hbar} \langle \psi | [\hat{H}_y, \hat{p}_y] | \psi \rangle = 0 \quad \text{since } [\hat{H}_y, \hat{p}_y] = 0$$

and the same for $\frac{d\langle \hat{p}_y^2 \rangle}{dt} \Rightarrow \; = 0$

e) From question c) and d) we have

$\Delta p_y \approx \frac{h}{d}$, and that it stays constant in time.

Consequently, a well-localized particle (in y-direction) will become delocalized according to

$$W \approx \Delta y \approx \frac{\Delta p_y}{m} \cdot t_1 \Rightarrow$$

$$W \approx \frac{h \cdot t_1}{d\, m} \quad \text{as soon as } W \gg d$$

(the relation does not hold yet at times short after passing the screen when $\frac{ht}{dm} \lesssim d$.)

f) $$\bar{\Psi}(y) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \Psi(y)\, e^{-ik_y y}\, dy$$

$$= \frac{1}{\sqrt{2\pi}} \int_{y_1 - d/2}^{y_1 + d/2} A_y e^{-ik_y y} dy = \frac{1}{ik_y \sqrt{2\pi}} \left[A_y e^{-ik_y y} \right]_{y_1 - d/2}^{y_1 + d/2}$$

$$= \frac{d A_y}{\sqrt{2\pi}} \frac{\sin\left(\frac{d}{2} k_y\right)}{\frac{d}{2} k_y} \cdot \underbrace{e^{-iy_1 k_y}}_{\substack{\text{phase shift of the state} \\ \text{in } k_y\text{-representation as} \\ \text{compared to b)}}}$$

A shift in real space (y-direction) gives a global phase shift for the state in k_y representation. $\Rightarrow$ It does not give any observable changes when measuring $\hat{p}_y$ properties.

Problem 4

7/8

a) The energy eigenvalues are the solutions of the time-independent Schrödinger equation

$\hat{H}_0|\varphi_i\rangle = E_i|\varphi_i\rangle$

In matrix notation this gives

$$\begin{pmatrix} E_0 & 0 \\ 0 & E_0 \end{pmatrix}\begin{pmatrix} 1 \\ 0 \end{pmatrix} = E_0\begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad \text{and} \quad \begin{pmatrix} E_0 & 0 \\ 0 & E_0 \end{pmatrix}\begin{pmatrix} 0 \\ 1 \end{pmatrix} = E_0\begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

indeed two consistent solutions for E_i and $|\varphi_i\rangle$.
A two-state system (and a 2x2 Hamiltonian matrix) has at most 2 different eigenvalues, and 2 eigenvectors

b) The two energy eigenvectors have the same eigenvalue E_0 $\Rightarrow$ E_0 is two-fold degenerate.

c) Now consistent solutions (again two solutions) of $\hat{H}|\varphi_i\rangle = E_i|\varphi_i\rangle$ are

$$\begin{pmatrix} E_0 & T \\ T & E_0 \end{pmatrix} \underbrace{\begin{pmatrix} 1/\sqrt{2} \\ 1/\sqrt{2} \end{pmatrix}}_{|\psi_1\rangle} = \underbrace{(E_0 + T)}_{\text{eigenvalue}} \underbrace{\begin{pmatrix} 1/\sqrt{2} \\ 1/\sqrt{2} \end{pmatrix}}_{|\psi_1\rangle}$$

$$\begin{pmatrix} E_0 & T \\ T & E_0 \end{pmatrix} \underbrace{\begin{pmatrix} 1/\sqrt{2} \\ -1/\sqrt{2} \end{pmatrix}}_{|\psi_2\rangle} = \underbrace{(E_0 - T)}_{\text{eigenvalue}} \underbrace{\begin{pmatrix} 1/\sqrt{2} \\ -1/\sqrt{2} \end{pmatrix}}_{|\psi_2\rangle}$$

8/8

d) See c), eigenvalues are

$E_0 + T$ (excited state, since $T > 0$)

$E_0 - T$ (ground state)

e) Normalized if $\langle\psi_1|\psi_1\rangle = 1$ $\Rightarrow$

$$\frac{1}{\sqrt{2}}\cdot\left(\langle\varphi_L| + \langle\varphi_R|\right)\cdot\left(|\varphi_L\rangle + |\varphi_R\rangle\right)\cdot\frac{1}{\sqrt{2}}$$

$$= \frac{1}{2}\left(\langle\varphi_L|\varphi_L\rangle + \langle\varphi_R|\varphi_R\rangle + \langle\varphi_L|\varphi_R\rangle + \langle\varphi_R|\varphi_L\rangle\right)$$

with $\langle\varphi_L|\varphi_L\rangle = \langle\varphi_R|\varphi_R\rangle = 1$ and

$\langle\varphi_L|\varphi_R\rangle = \langle\varphi_R|\varphi_L\rangle = 0$ since

$|\varphi_L\rangle$ and $|\varphi_R\rangle$ are orthonormal eigenvectors of $\hat{H}_0$ $\Rightarrow$ $\langle\psi_1|\psi_1\rangle = 1$

f) The system is the no longer in an energy eigen state of the Hamiltonian $\Rightarrow$ The expectation value for the observable that describes the position (which must commute with $\hat{H}_0$) will oscillate in time $\Rightarrow$ The position of the electron oscillates between the two wells.

g) System is then again in an eigen state of the Hamiltonian $\Rightarrow$ Is a stationary state $\Rightarrow$ No expectation value of any observable depends on time. The system is and stays in the ground state $|\psi_2\rangle = \frac{|\varphi_L\rangle - |\varphi_R\rangle}{\sqrt{2}}$.