

FROM:

Problem set for 3rd week of the course Quantum Physics 1 For the tutorial sessions of 17 and 19 September 2014

Homework, to be made before the werkcollege:

From the book (Griffiths 2nd Ed.) Chapter 2 - 2.18, 2.19 (just use the result stated in problem 1.14. if you did not yet make that problem), 2.21 and from Chapter 3 - 3.1, 3.3, 3.22.

Problems to work on during werkcollege:

Problems W3.1 – W3.5 (this hand out) and from the book Chapter 3 - 3.5, this is the minimal set you need to do. Other good problems that we selected (we advise you to make these for the topics where you need or like to do extra training):

from the book Chapter 2 - 2.20, and from Chapter 3 - 3.2, 3.4, 3.21, 3.23 (work this problem also out by using a matrix representation that uses the basis that is spanned by the vectors $|1\rangle$ and $|2\rangle$), 3.24.

NOTE: Fourier transform relations between x - and k -representation of a state:

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

Problem W3.1

This problem (about a particle in a box) is meant to clarify how the same state of quantum system can be *represented* in many different ways. The representations and notations that will be used here are:

- describing a state using Dirac notation.
- a wavefunction that is a function of position x .
- a wavefunction that is a function of wave number k (or, equivalently, momentum $p_x = \hbar k$).
- a superposition of energy eigenstates.

On the way, you will practice with Fourier transforms and decomposition of a state into eigenvectors.

a) The particle in the box is modeled as a particle in an infinitely deep potential well with $V=0$ for $|x| < a/2$, and $V=\infty$ elsewhere. The particle is brought into the box with a mechanism that results in a wavefunction for the particle that is evenly distributed in the well, $\Psi(x) = 1/\sqrt{a}$ for $|x| < a/2$ and zero elsewhere. Represent this state in the k -representation (hint: you need to Fourier transform the state).

b) Alternatively, this state can for example be represented as a superposition of energy eigenstates of the system in Dirac notation, $|\Psi\rangle = \sum_n c_n |\varphi_n\rangle$. We will use this later in this problem. In this question we first pay attention to the relation between the x -representation and the representation with Dirac notation. Prove the relation $\Psi(x) = \langle x | \Psi \rangle$ (here $|x\rangle$ is the eigenvector with eigenvalue x for the position operator \hat{x} , which means that the state $|x\rangle$ in Dirac notation corresponds to $\delta(x' - x)$ in x -representation, see also Griffiths p. 70 [Sec. 2.5], 104-105 [Sec. 3.3]).

c) Eq. [2.28] of the Griffiths book ($\psi_n(x)$ in Sec. 2.2) gives the energy eigenstates for a particle in this system, but for a box (or quantum well) that runs from $x=0$ to $x=a$. Here we use a description where the box runs from $x=-a/2$ to $x=a/2$ (and slightly different notation with $\varphi_n(x)$ for the energy eigenstates, instead of $\psi_n(x)$ as in the book). The energy eigenvalues E_n are of course the same, but the eigenstates are now

$$\varphi_n(x) = \sqrt{\frac{2}{a}} \cos\left(\frac{n\pi x}{a}\right), \quad \text{for } n = 1, 3, 5, 7, \dots$$
$$\varphi_n(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right), \quad \text{for } n = 2, 4, 6, 8, \dots$$

Write down the eigenfunctions for odd n in the k -representation (you need to use the Fourier transform, see also Griffiths p. 61-62 [Sec. 2.4], and 108 [Sec. 3.4]).

d) Sketch the wavefunction of the particle (for the state as in question **a**), as well as the energy eigenstates $|\varphi_1\rangle$ and $|\varphi_9\rangle$ in the k -representation. Explain the differences between the graphs.

Hint 1: you need to sketch here a *sinc function* or the sum of two shifted *sinc functions*. In its most basic form the sinc function is $\text{sinc}(x) = \sin(x)/x$. It is easy to construct as follows: Sketch $\sin(x)$, sketch $1/x$, and multiply the two graphs. Also look up the value of the limit of $\sin(x)/x$ for $x \rightarrow 0$ (see for example Griffiths p. 62-64 [Sec. 2.4]).

Hint 2: for $\Psi(x)$ in k -representation write it in the form of a sinc function. For $|\varphi_1\rangle$ and $|\varphi_9\rangle$ in k -representation, try to write this as the sum of two shifted sinc functions. That is, for $n = 1$ and $n = 9$ your answer should have a term that contains the factor $\text{sinc}\left(\left(k - \frac{n\pi}{a}\right)\frac{a}{2}\right)$ and a term that contains the factor $\text{sinc}\left(\left(k + \frac{n\pi}{a}\right)\frac{a}{2}\right)$.

e) For continuing on **b**), you need to determine the coefficients c_n for odd n . Prove the relation $c_n = \langle \varphi_n | \Psi \rangle$ in Dirac notation (this quantity c_n is often called the projection of $|\Psi\rangle$ onto $|\varphi_n\rangle$).

f) Evaluate the inner product $c_n = \langle \varphi_n | \Psi \rangle$ for odd n in the x -representation.

g) Write down the inner product $c_n = \langle \varphi_n | \Psi \rangle$ for odd n in the k -representation, but only solve the integral if you feel like doing so.

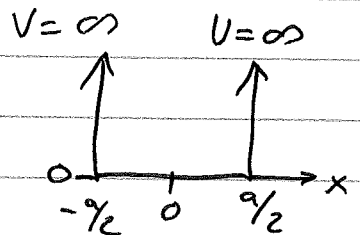
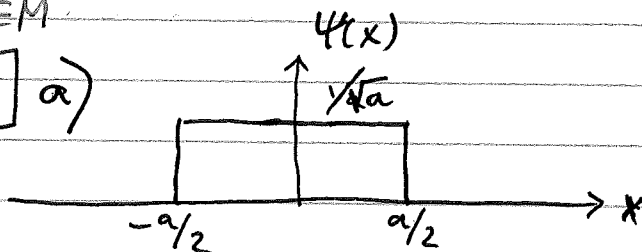
h) Without doing the calculation, can you say what the value is of $c_n = \langle \varphi_n | \Psi \rangle$ for even n .

Answers for problems Quantum Physics 1
Problemset for **WEEK 3** of the course

(Correction: The answers of problem 5.9 of last week will not be presented. 5.9 was also replaced by problems W4.1 and W4.2 of last week.)

PROBLEM

W3.1 a)



$$\bar{\Psi}(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-ikx} \psi(x) dx = \frac{1}{\sqrt{2\pi}} \frac{1}{\sqrt{a}} \int_{-a/2}^{a/2} e^{-ikx} dx$$

$$= \frac{1}{\sqrt{2\pi a}} \left[\frac{1}{-ik} e^{-ikx} \right]_{-a/2}^{a/2} \Rightarrow$$

$$\bar{\Psi}(k) = \frac{2\sqrt{a}}{\sqrt{2\pi}} \frac{\sin(\frac{a}{2}k)}{ak}$$

$\lim_{k \rightarrow 0} = \frac{\sqrt{a}}{\sqrt{2\pi}}$

$$= \frac{\sqrt{a}}{\sqrt{2\pi}} \frac{\sin(\frac{a}{2}k)}{\frac{a}{2}k}$$

see p. 70 book

b) $\langle x | \Psi \rangle = \int_{-\infty}^{\infty} \delta(x'-x) \Psi(x') dx' = \Psi(x)$

c) $\varphi_n(x) = \sqrt{\frac{2}{a}} \cos\left(\frac{n\pi x}{a}\right)$ for odd n

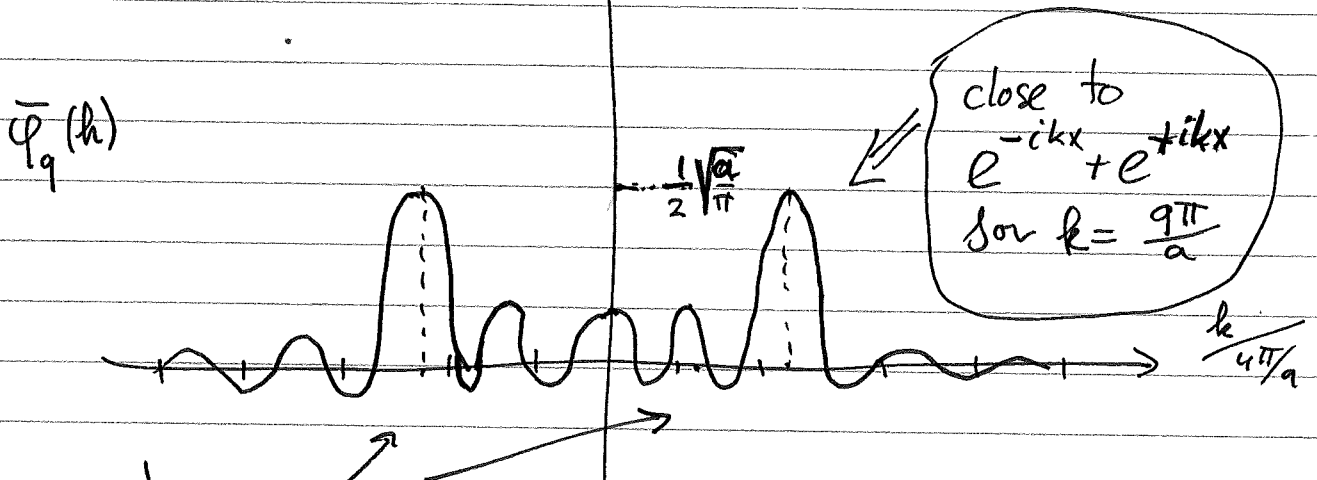
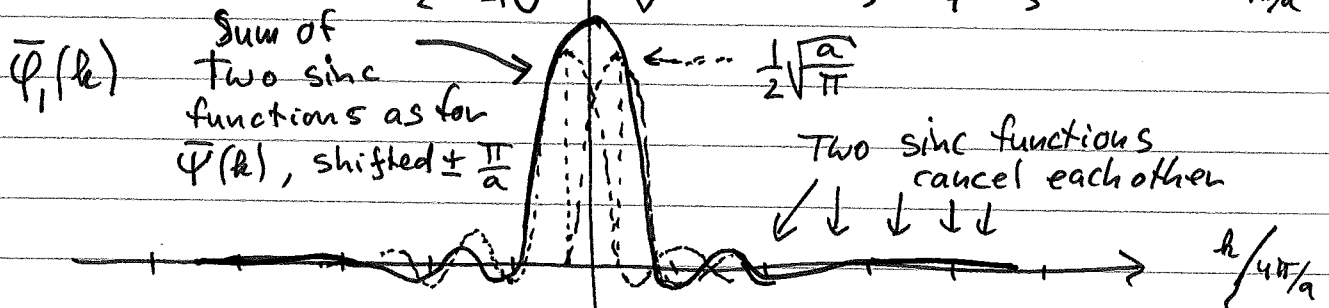
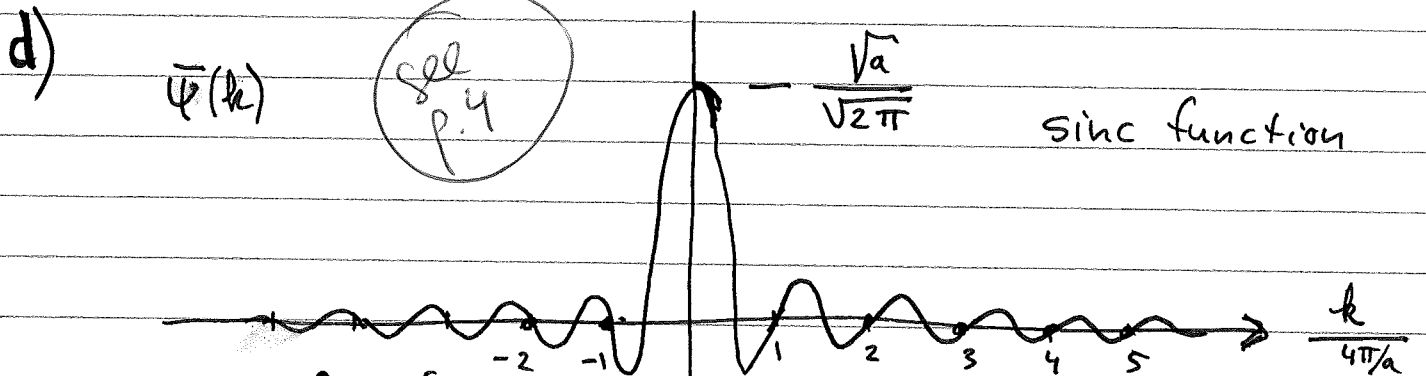
$$\bar{\varphi}_n(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-ikx} \varphi_n(x) dx =$$

$$= \frac{1}{\sqrt{a\pi}} \frac{1}{2} \int_{-a/2}^{a/2} \left(e^{in\pi x/a} + e^{-in\pi x/a} \right) e^{-ikx} dx$$

$$= \frac{1}{\sqrt{a\pi}} \frac{1}{2} \int_{-a/2}^{a/2} \left(e^{-i(k - \frac{n\pi}{a})x} + e^{-i(k + \frac{n\pi}{a})x} \right) dx$$

$$= \frac{1}{\sqrt{a\pi}} \frac{1}{2} \left(\left[\frac{1}{-i(k - \frac{n\pi}{a})} e^{-i(k - \frac{n\pi}{a})x} \right]_{-a/2}^{a/2} + \left[\frac{1}{-i(k + \frac{n\pi}{a})} e^{-i(k + \frac{n\pi}{a})x} \right]_{-a/2}^{a/2} \right)$$

$$\bar{\varphi}_n(k) = \frac{1}{2} \cdot \frac{\sqrt{a}}{\sqrt{\pi}} \left(\frac{\sin\left(\left(k - \frac{n\pi}{a}\right) \cdot \frac{a}{2}\right)}{\left(k - \frac{n\pi}{a}\right) \cdot \frac{a}{2}} + \frac{\sin\left(\left(k + \frac{n\pi}{a}\right) \cdot \frac{a}{2}\right)}{\left(k + \frac{n\pi}{a}\right) \cdot \frac{a}{2}} \right)$$



Sum of two sinc functions as for $\bar{\varphi}(k)$, shifted by $\pm \frac{9\pi}{a}$

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$$e) \langle \varphi_n | \Psi \rangle = \langle \varphi_n | \left(\sum_{n'} c_{n'} | \varphi_{n'} \rangle \right)$$

$$= \sum_{n'} c_{n'} \langle \varphi_n | \varphi_{n'} \rangle$$

$$\langle \varphi_n | \varphi_{n'} \rangle = \begin{cases} 0, & n \neq n' \\ 1, & n = n' \end{cases}$$

$$= c_n \langle \varphi_n | \varphi_n \rangle = c_n$$

$$f) \langle \varphi_n | \Psi \rangle = \int_{-\infty}^{\infty} \varphi_n^*(x) \Psi(x) dx$$

$$= \int_{-a/2}^{a/2} \frac{1}{\sqrt{a}} \sqrt{\frac{2}{a}} \cos\left(\frac{n\pi x}{a}\right) dx = \frac{\sqrt{2}}{n\pi} \left[\sin\left(\frac{n\pi x}{a}\right) \right]_{-a/2}^{a/2} \Rightarrow$$

$$c_n = (-1)^{\frac{n+3}{2}} \cdot \frac{2\sqrt{2}}{n\pi} \Rightarrow |\Psi\rangle = \sum_n (-1)^{\frac{n+3}{2}} \frac{2\sqrt{2}}{n\pi} |\varphi_n\rangle$$

→ for n = 1, 3, 5, 7 etc.

$$g) \langle \varphi_n | \Psi \rangle = \int_{-\infty}^{\infty} \bar{\varphi}_n^*(k) \bar{\Psi}(k) dk$$

$$= \frac{1}{\pi} \int_{-\infty}^{\infty} \left(\frac{\sin\left(\frac{a}{2}\left(k - \frac{n\pi}{a}\right)\right)}{\left(k - \frac{n\pi}{a}\right)} + \frac{\sin\left(\frac{a}{2}\left(k + \frac{n\pi}{a}\right)\right)}{\left(k + \frac{n\pi}{a}\right)} \right) \frac{\sin\left(\frac{a}{2}k\right)}{ak} dk$$

Sometimes x-representation is more convenient, sometimes k-representation!

h) All $c_n = 0$ for n odd even number.

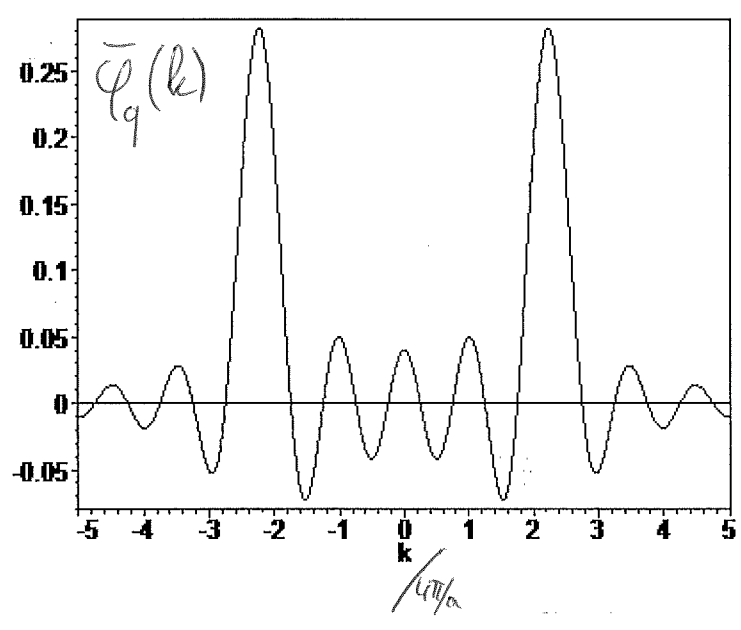
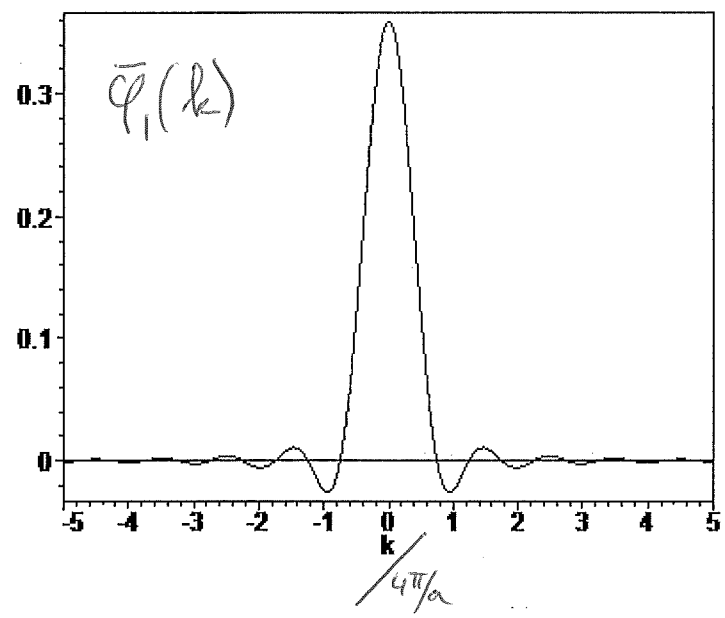
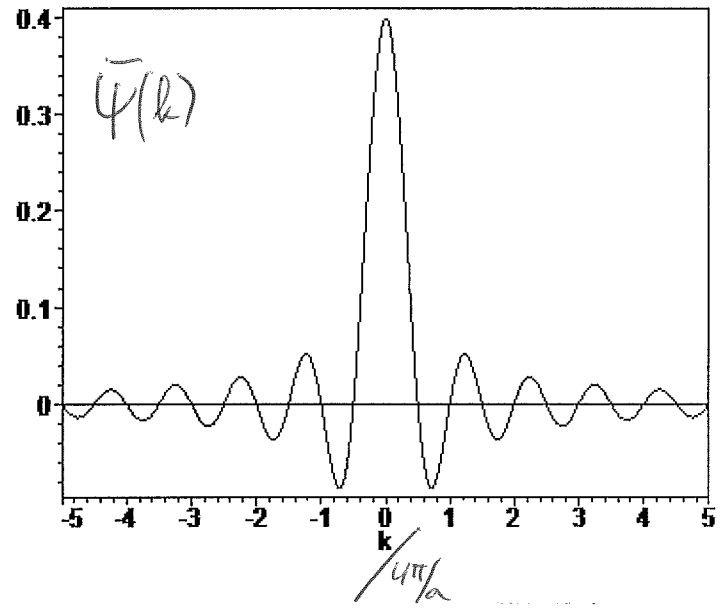
Inner product $\left(\int_{-a/2}^{a/2} \varphi_n^*(x) \Psi(x) dx \right)$ is zero,

because $\Psi(x)$ is an even function, and

all the $\varphi_n(x)$ for even n are odd functions

plotted for $a=1$

extra for W3.1 (or CS.1 d)



For higher k less contribution in $\bar{\psi}_1(k)$ as compared to $\bar{\psi}(k) \Rightarrow$ \square has more high frequencies than \sim

In $\bar{\psi}_9(k)$ more contributions for $\pm \approx 2.5 k/\pi/a \Rightarrow$ similar to plane waves in + and - direction with these k -values