# 4. HOMEWORK SHEET FOR QUANTUM MECHANICS To be handed in on the 5.5 in the tutorial

## $\mathbf{Q}$ **10**: Change of basis

### (10 points)

We consider the discretisation of a wave function of a force free particle (in 1D)  $\psi(x)$  on a finite, 1D grid/lattice with  $N \in \mathbb{N}$  lattice points (N is an even integer) and a lattice spacing of  $\Delta x = a$ . The following relations are given:

Continuous description	discrete, finite in 1D
Eigenvalue of the position operator	
x	ma , $m = 0, 1,, N - 1$
Eigenfunction of the position operator	
x angle	$\frac{ m\rangle}{\sqrt{a}}$
	·
Wave function in position space	
$\psi(x)$	$\frac{\psi_m}{\sqrt{a}}$
	V u
Eigenvalue of the momentum operator	
р	$\left  \frac{2\pi\hbar}{Na} l \right ,  l = -\frac{N}{2}, -\frac{N}{2} + 1, \dots, \frac{N}{2} - 1$
Eigenfunction of the momentum operator p	
p angle	$\sqrt{rac{Na}{2\pi\hbar}}\ket{l}$

The change of basis from the basis  $\{|m\rangle\}$  to the basis  $\{|l\rangle\}$  is described by the function

$$f_l(m) = \langle m|l \rangle = \frac{1}{\sqrt{N}} \exp\left(i\frac{2\pi}{Na}lma\right) \qquad (*)$$

with m = 0, 1, 2, ..., N - 1 and  $l = -\frac{N}{2}, -\frac{N}{2} + 1, ..., \frac{N}{2} - 1$ 

- a) Show that  $f_l(m)$  is periodic in l as well as in m, with the period N. (1 point)
- b) Show that  $\sum_{l} f_{l}^{*}(m) f_{l}(m') = \delta_{mm'}$  (Completeness of  $f_{l}(m)$ ). (2 points)
- c) Show that  $\sum_{m} f_l^*(m) f_{l'}(m) = \delta_{ll'}$  (Orthogonality of  $f_l(m)$ ). (2 points)
- d) In the basis  $\{|l\rangle\}$  the momentum operator is represented by the diagonal matrix

$$\langle l | \hat{p} | l' \rangle \, = \, \frac{2\pi\hbar}{Na} \, l \, \delta_{ll'}.$$

Calculate the matrix elements  $\langle m | \hat{p} | n \rangle$  of the momentum operator in the basis  $\{|m\rangle\}$ . Consider the limit  $a \to 0$ ,  $N \to \infty$  and show that one gets the famous result  $\langle x | \hat{p} | x' \rangle = \frac{\hbar}{i} \delta'(x - x')$ . Briefly discuss the connection between (\*) and the Fourier transformation. (5 points)

**Q 11**: *1D problem: infinitely deep potential well* Consider the 1D, infinitely deep potential well

$$V(x) = \begin{cases} 0 & \text{for } 0 < x < L \\ +\infty & \text{otherwise.} \end{cases}$$

- a) Determine the (normalised to unity) solution to the corresponding time independent Schrodinger equation, i.e. determine the normalised Eigenfunction  $\psi(x)$  and the corresponding Eigenvalues E of the corresponding Hamiltonian operator  $\hat{H}$ . (2 points) Tip: Use the boundary conditions for an infinitely high potentialwell (see Q 9 c).
- b) Calculate for the Eigenfunction of a) the expectation of position and momentum as well as the mean squared deviation.(3 points)
- c) Now determine the normalised Eigenfunctions of  $\hat{H}$  for the potential

$$V(x) = \begin{cases} 0 & \text{for } -L/2 < x < L/2 \\ +\infty & \text{otherwise,} \end{cases}$$

so that the reflection symmetry at x = 0 is obvious (most easily done using the solutions of a)). How are the energy Eigenvalues different? How are the expectation values of the position and momtentum, as well as their root mean square different? (3 points)

#### Q 12: Probability density current

(2 points)

The wavefunction  $\psi(\vec{x}, t)$  provides the probability density

$$\rho(\vec{x},t) = |\psi(\vec{x},t)|^2,$$

that that a particle is in position  $\vec{x}$ , i.e.  $\rho(\vec{x}, t)d^3\vec{x}$  is the probability to find a particle at position  $\vec{x}$  in a volume element  $d^3\vec{x}$ .

Show with help of the time dependent Schrödinger equation for a particle in a potential  $V(\vec{x})$ , that  $\rho(\vec{x}, t)$  satisfies the continuity equation

$$\frac{\partial}{\partial t}\rho(\vec{x},t) \,+\, \vec{\nabla}\cdot\vec{j}(\vec{x},t) = 0$$

with the probability current

$$\vec{j}(\vec{x},t) \, := \, \frac{i\hbar}{2m} \left[ \psi(\vec{x},t) \, \vec{\nabla} \psi^*(\vec{x},t) \, - \, \psi^*(\vec{x},t) \vec{\nabla} \psi(\vec{x},t) \right].$$

#### Ganz ungebunden

Niels BOHR erhielt einen Brief von PAULI, den zu beantworten ihm schwer fiel. Er bat seine Frau, PAULI zu schreiben, er selbst werde ihm am Montag schreiben. Zwei Wochen später schrieb PAULI an Frau Bohr, wie weise BOHR gewesen sei, als er hatte mitteilen lassen, er werde Montag schreiben, aber nicht an welchem. Er brauche sich keineswegs an Montag gebunden zu fühlen.

Aus: Anna Ehlers, Liebes Hertz !, Physiker und Mathematiker in Anekdoten, Birkhäuser Verlag, 1994, S. 47

(8 points)