Übungen zur Modernen Theoretischen Physik I – English Sheet –

Prof. Dr. Gerd Schön	Sheet 6
Andreas Heimes, Dr. Andreas Poenicke	Besprechung 11.06.2014

1. Benzene

(3 points)

(2 points)

A benzene ring is composed of six carbon atoms. This system can be modeled as singleparticle levels with energy ε coupled by a hopping amplitude t. In the local basis $\{|n\rangle\} = \{|0\rangle, |1\rangle, ..., |5\rangle\}$, where $|n\rangle$ denotes the localized state on the nth atom, the Hamiltonian reads

$$\hat{H} = t \sum_{n=0}^{5} \left(\left| n+1 \right\rangle \left\langle n \right| + \left| n \right\rangle \left\langle n+1 \right| \right) + \varepsilon \sum_{n=0}^{5} \left| n \right\rangle \left\langle n \right| \,,$$

with the periodic boundary condition $|0\rangle = |6\rangle$. Determine the eigenvalues and eigenvectors in the basis $\{|n\rangle\}$.

[Hint: Diagonalize the Hamiltonian, using the Fourier representation, i.e. $|k\rangle = \frac{1}{\sqrt{6}} \sum_{n=0}^{5} e^{ikn} |n\rangle$.]



2. Baker-Hausdorff Formula

It is given that \hat{A} and \hat{B} commute with the commutator $[\hat{A}, \hat{B}]$, i.e. $[\hat{A}, [\hat{A}, \hat{B}]] = 0$ and $[\hat{B}, [\hat{A}, \hat{B}]] = 0$. Show, that in this case

$$e^{\hat{A}+\hat{B}} = e^{\hat{A}}e^{\hat{B}}e^{-\frac{1}{2}[\hat{A},\hat{B}]}.$$

[Hint: Define an operator $\hat{T}(\lambda) := e^{\hat{A}\lambda}e^{\hat{B}\lambda}$ and consider $\frac{\partial \hat{T}(\lambda)}{\partial \lambda}$. Use the relation $[\hat{B}, \hat{A}^n] = n\hat{A}^{n-1}[\hat{B}, \hat{A}]$ (s. Sheet 5, Ex. 3d) to calculate the commutator $[\hat{B}, e^{-\hat{A}\lambda}]$.]

3. Measurement

(5 Punkte)

A qubit (quantum **bit**) is a quantum-mechanical two-level system. We have seen an example in exercise 2 c) of sheet three, where we were discussing the double-well potential. In the basis of the energetically lowest eigen-states of this system, $\{|1\rangle, |2\rangle\}$, the Hamiltonian can be written as

$$\hat{H} = \begin{pmatrix} E_1 & 0\\ 0 & E_2 \end{pmatrix} = \frac{E_1 + E_2}{2} \mathbb{1} + \frac{E_1 - E_2}{2} \hat{\sigma}_z = \varepsilon \mathbb{1} - \frac{\delta \varepsilon}{2} \hat{\sigma}_z, \tag{1}$$

where $\mathbbm{1}$ is the $2\times 2\text{-unit}$ matrix and

$$\hat{\sigma}_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \hat{\sigma}_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \qquad \hat{\sigma}_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \tag{2}$$

are the Pauli-matrices.

It is given that the qubit is initialized in the state $|\psi\rangle = \alpha |1\rangle + \beta |2\rangle$.

- (a) [1 point] Calculate the expectation value for the energy $\langle \hat{H} \rangle$ and the standard-deviation $\Delta E = \sqrt{\langle \hat{H}^2 \rangle \langle \hat{H} \rangle^2}$.
- (b) [1 point] Now we measure the observable $\hat{A} = \hat{\sigma}_x$. What values can be measured and what is the corresponding probability? What is the corresponding state right after the measurement?
- (c) [1 point] Right after the measurement in (b) the energy \hat{H} is measured. Again determine the measurement-value and the corresponding probability.
- (d) [2 points] Now the qubit will be initialized in the ground-state $|1\rangle$. The observables $\hat{B} = \hat{\sigma}_y$ and $\hat{A} = \hat{\sigma}_x$ will be measured one right after the other in the order \hat{B} then \hat{A} . What are the possible measurement results and what are the corresponding probabilities?