GEORG-AUGUST-UNIVERSITÄT
GÖTTINGEN

Fakultät für
Physik

Bachelor's Thesis

Hier steht das Thema der Arbeit in deutsch

Here comes the title of the thesis in english

prepared by

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Abstract

Here the key results of the thesis can be presented in about half a page.

Keywords: Physics, Bachelor thesis

Zusammenfassung

Hier werden auf einer halben Seite die Kernaussagen der Arbeit zusammengefasst.

Stichwörter: Physik, Bachelorarbeit

Contents

Nomenclature

Lateinische Buchstaben

Variable	Bedeutung	Einheit
A	Querschnittsfl"ache	m^2
c	Geschwindigkeit	$^{\mathrm{m}}/_{\mathrm{s}}$

Griechische Buchstaben

Variable	Bedeutung	Einheit
α	Winkel	$^\circ$; –
ϱ	Dichte	$^{\mathrm{kg}}/_{\mathrm{m}^3}$

Indizes

Index	Bedeutung
m	Meridian
r	Radial

Abk"urzungen

Abk"urzung	Bedeutung
2D	zweidimensional
3D	dreidimensional
max	maximal

1. Einleitung

Diese Vorlage `GAUBM` für Bachelor- bzw. Masterarbeiten ist eine Überarbeitung der Vorlage von Simon Dreher für Abschlußarbeiten am Institut für Mikrosystemtechnologie (IMTEK) an der Universität Freiburg. Die eigentliche Datei mit der Klassendefinition ist `GAUBN.cls`, die Sie zusammen mit dieser Datei erhalten haben. Weitere Dateien sind `datenumber.sty` und die zugehörigen Sprachdefinitionen `\datenumber*.ldf`. Im Verzeichnis `figures` finden sich die von der Klasse benötigten Logos (Universität und Physik) sowie Beispielbilder für die Übersetzung dieser Beispieldatei (`bthesis.tex`). Sie können diese Datei als Vorlage für Ihre Arbeit nutzen und entsprechend modifizieren. Bitte denken Sie daran, sie vorher unter einem eigenen Namen abzuspeichern. Um die Datei anzupassen, gehen Sie wie folgt vor:

Bei den Parametern zu `\documentclass[...]{GAUBM}` in der Präambel kann man durch Umschalten zwischen `english,ngerman` und `ngerman,english` eine deutsche Arbeit (erste Variante) mit Englisch als Alternativsprache bzw. eine englische Arbeit (zweite Variante) mit deutsch als Alternativsprache wählen. Im laufenden Text kann man mit

```
\begin{otherlanguage}{english/ngerman}
...
\end{otherlanguage}
```

zur alternativen Sprache wechseln.

Nach `\begin{document}` müssen zuerst ein paar Befehle mit Information über die Arbeit aufgerufen werden:

1. `\ThesisAuthor{Vorname}{Nachname}`: Die Argumente sind der Vorname und Nachname der Autorin bzw. des Autors der Arbeit.

2. `\PlaceOfBirth{Wohnort}`: Der Geburtsort der Autorin bzw. des Autors.

3. `\ThesisTitle{Deutscher Titel}{English title}`: Der deutsche und englische Titel der Arbeit gemäß Antrag.

4. `\Institute{Institut}`: Das Institut, an dem die Arbeit angefertigt wurde.

5. `\FirstReferee[Betreuer/in]{Erste/r Gutachter/in}`: Voller Titel und Name des/r Erstgutachter/in. Ist der Betreuer der Arbeit *nicht* identisch mit dem/r Erstgutachter/in, so muß der volle Titel und der Name des/r Betreuer/in als optionales Argument in eckigen Klammern erscheinen.

6. `\SecondReferee{Zweite/r Gutachter/in}`: Voller Titel und Name des/r Zweitgutachter/in.

7. `\ThesisBegin{Tag}{Monat}{Jahr}`: Datum des Beginns der Anfertigung der Arbeit gemäß Antrag.

8. `\ThesisEnd{Tag}{Monat}{Jahr}`: Datum der Fertigstellung der Arbeit.

9. Optional kann mit

   ```
   \begin{abstract}
   ...
   \end{abstract}
   ```

   eine maximal eine halbe Seite lange Zusammenfassung eingefügt werden.

   Falls man die Zusammenfassung in der alternativen Sprache verfassen möchte, dann geht das mit der Befehlsfolge

   ```
   \begin{otherlanguage}{english/ngerman}
   \begin{abstract}
   ...
   \end{abstract}
   \end{otherlanguage}
   ```

2. Grundlagen

In diesem Kapitel werden die theoretischen Grundlagen erläutert.

Wichtige Gleichungen, die in der Arbeit häufiger zitiert werden, sollten eine Gleichungsnummer erhalten.

$$a^2 + b^2 = c^2 \tag{2.1}$$

Zum Beispiel wird in Gleichung 2.1 der Satz des Pythagoras angegeben.

Gerade im Bereich der Grundlagen wird viel Literatur zitiert, z.B. [**?**]. Falls mehrere Literaturzitate auf einmal zitiert werden, ist folgendes z.B. möglich [**? ? ? ?**].

2.1. Unterkapitel Gliederungsebene 2

Hier sollte etwas Text stehen.

2.1.1. Unterkapitel Gliederungsebene 3

Noch ein paar Beispiele zu Abbildungen und Tabellen:

Abbildung 2.1 verdeutlicht ...

Wie die Abb. 2.1 und Tab. 2.1 verdeutlichen ...

Text...

Text...

A-Wert	*B*-Wert	*C*-Wert	*D*-Wert
aaaaaa	bbbbbbb	cccccc	ddddddd
aaaaaa	bbbbbbb	cccccc	ddddddd

Table 2.1.: Tabellenbeschreibung

Figure 2.1.: Bildbeschreibung

3. “Lab course”

3.1. Theoretical foundation and numerical methods

3.1.1. Introduction, exact diagonalization

In what follows, we are interested in a one-dimensional XXZ Heisenberg chain with next-nearest neighbour coupling. As such, we consider the following Hamiltonian:

$$H(J,\mu) = H_1(J,\mu) + \lambda H_2(J,\mu), \tag{3.1}$$

$$H_n(J,\mu) = J\sum_{i=1}^{N}\left[\frac{1}{2}\left(S_i^+ S_{i+n}^- + S_i^- S_{i+n}^+\right) + \mu S_i^z S_{i+n}^z\right], \tag{3.2}$$

where the spins are labeled $i = 1,\ldots,N$ and J is the interaction constant. The scalar product for the spin operators $\mathbf{S}_i \cdot \mathbf{S}_{i+n}$ has been decomposed into creation-annihilation operators $S^{\pm} = S^x \pm iS^y$ while μ introduces an anisotropy for the z-direction compared to the x and y directions. Finally, λ is a parameter controlling the strength of the next-nearest neighbor (NNN) interactions cf. [1, 4ff.].
First, would like to numerically compute the time evolution of such a system by means of exact diagonalization.

3.1.2. Block diagonalization

In the following section, we follow closely the techniques and notation from [4, 55ff.]. The states are denoted as $|S_0^z, S_1^z, \ldots, S_{N-1}\rangle$, where the subscript $i = 0,\ldots,N-1$ refers to the site i of our one-dimensional chain. A particular state is abridgedly labeled by arrows, e.g. $|\uparrow\downarrow\uparrow\downarrow\ldots\rangle$. Furthermore, periodic boundary conditions, which add additional symmetries, are assumed ($i = N-1+n \equiv n-1$). Exact diagonalization allows for total knowledge of the properties of a finite system by choosing a basis, setting up a Hamiltonian and diagonalizing it numerically. While theoretically applicable to any system size, this method is limited to around 30 spins,

as the computational cost for diagonalization is $\propto 8^{\text{dim. of basis}}$[citation needed.] and the spin basis above grows like 2^N without utilizing symmetries. Symmetries can be used to transform the Hamiltonian matrix into block-diagonal form cf. [4, 56] with each block belonging to states with a conserved quantum number, thereby reducing the basis dimension. In this first chapter, only the conservation of z-component of the total spin ($\hat{=}$ total magnetization) $m_z = \sum_{i=0}^{N-1} S_i^z$ is used:
It is easy to verify, using the usual commutation relations for the spin operators [citation needed] that

$$[S_i^z, H] = \frac{1}{2}(A_1 + A_2), \tag{3.3}$$

$$A_n = S_i^+ S_{i+n}^- - S_i^- S_{i+n}^+ - S_{i-n}^+ S_i^- + S_{i-n}^- S_i^+. \tag{3.4}$$

By using the periodic boundary conditions it follows that

$$\sum_{i=0}^{N-1} A_n = \sum_{i=0}^{N-1} \left(S_i^+ S_{i+n}^- - S_i^- S_{i+n}^+\right) - \underbrace{\sum_{i=n}^{N-1+n}}_{\equiv \sum_{i=0}^{N-1}} \left(S_i^+ S_{i+n}^- - S_i^- S_{i+n}^+\right) = 0, \tag{3.5}$$

and therefore

$$[H, m_z] = 0, \tag{3.6}$$

meaning that m_z is a conserved quantity. By constructing a basis with fixed magnetization, blocks of size $M \times M$ with the same m_z can be considered independently. M is the fixed magnetization basis dimension: [4, 60]

$$M = \frac{N!}{n_\uparrow!\; n_\downarrow!}. \tag{3.7}$$

3.1.3. Bit representation

As Spin-1/2 partlicles only have two possible states ($\uparrow$ & $\downarrow$), they can be elegantly represented in a computer via the bits “1” and “0”. More precisely, A lattice state $|S_0^z, S_1^z, \ldots, S_{N-1}\rangle$ is represented as the bit representation of an unsigned integer, with the first bit denoted by the index 0. [4, 59], e.g. $|\uparrow\downarrow\downarrow\uparrow\rangle \hat{=} 1001 \doteq 9$. Symmetries that will come in later, like spin translation or rotation manifest themselves as operations on these bit representations.

3.1.4. Construction of the fixed magnetization basis

A basis list of states having the same magnetization m_z is found by iterating over all integers s from the 2^n dimensional basis and counting the amount of "1" bits $n_\uparrow$, checking whether they amount to the target magnetization $m_z{=}n_\uparrow - N/2$.
With $s[i]$ labeling the i'th bit, starting from 0, the following pseudocode is used to obtain an ordered list of basis states s_a:

$a = 0$
for all $s = 0..2^N - 1$ **do**
  if $\sum_i s[i] = n_\uparrow$ **then**
    $a \leftarrow a + 1$
    $s_a \leftarrow s$
  end if
end for
$M \leftarrow a$

M is the basis dimension. Thus, in terms of M-tuples, a natural basis is given by all vectors

$$\hat{e}_a = (0, \ldots, 0, \underbrace{1}_{c_a}, 0, \ldots, 0)^T, a = 1..M, \tag{3.8}$$

each representing the corresponding integer state s_a.

3.1.5. Construction of the Hamilton matrix

The Hamiltonian (3.2) is translated into a matrix for the fixed magnetization basis cf. [4, 60f.]. The diagonal terms are $\langle a|S_i^z S_{i+n}^z|a\rangle = \pm 1/4\ \mu$,since the i'th and $i{+}n$'th spin are either equal or different. The off-diagonal terms $\left(S_i^+ S_{i+n}^- + S_i^- S_{i+n}^+\right)$ flip the bits i and $i+n$ $(0 \leftrightarrow 1)$ and amount to zero otherwise. A bisectional search [Pseudocode?] is used to find position b of the flipped state s^*, giving a matrix element contribution of $\langle b|(S_i^+ S_{i+n}^- + S_i^- S_{i+n}^+)|a\rangle = +1/2$. In pseudocode, the matrix belonging to the NNN Hamiltonian $(n = 1, 2)$ is constructed as follows:

for $a = 1..M$ **do**
  for $n = 1, 2$ **do**
    $j = (i + n) \mod N$

```
        if a[i] = a[j] then
            H(a,a) ← H(a,a) + 1/4 μ
        else
            H(a,a) ← H(a,a) − 1/4 μ
            s* = flipstate(a)
            b ← findstate(s*)
            H(a,b) = 1/2
        end if
    end for
end for
```

3.1.6. Diagonalization and time evolution

The Armadillo package [3] is used for matrix diagonalization and vector operations. After setting up the Hamilton matrix, the eigenvectors and eigenvalues are computed. Each eigenstate $|\lambda\rangle$ is a superposition of the natural spin states $|a\rangle = |\uparrow\downarrow\uparrow\uparrow \ldots \downarrow\rangle$, which themselves are represented by the bits of an integer. The vectors $\mathbf{c}$, which represent the states and have components c_a, are to be transformed into the eigenbasis. A general initial state $|\psi\rangle$ is decomposed in the eigenbasis as follows:

$$\begin{aligned} H|\psi\rangle &= \sum_a \sum_b |a\rangle \underbrace{\langle a|H|b\rangle}_{H_{ab}} \underbrace{\langle b|\psi\rangle}_{c_b} = \sum_a \sum_b \sum_\lambda |a\rangle \langle a|\lambda\rangle\langle\lambda|b\rangle \langle b|\psi\rangle \\ &= \sum_\lambda \lambda |\lambda\rangle \underbrace{\langle\lambda|\psi\rangle}_{c_\lambda}, \end{aligned} \tag{3.9}$$

where c_λ are the components of the vector $\mathbf{c}$ in the eigenbasis and λ are the eigenvalues (energies). The matrix elements and column vectors are what we actually work with. The natural spin states remain untouched.
We would now like to compute the time evolution of the system, which is done in the eigenbasis. Utilizing the time evolution operator $U(t) = e^{-iHt}$ it holds that

$$e^{-iHt}|\psi\rangle = e^{-iHt}\sum_\lambda c_\lambda |\lambda\rangle = \sum_\lambda \underbrace{e^{-i\lambda t}c_\lambda}_{c_\lambda(t)} |\lambda\rangle . \tag{3.10}$$

3.1.7. Measurements and observables

In light of the probabilistic nature of quantum mechanics, we are interested in measuring the expectation value of an observable $\langle O \rangle$. Another important quantity later on will be the Loschmidt echo M [2], which is generally defined as

$$M(t) = \left| \langle \psi_0 | e^{iH_2 t} e^{-iH_1 t} | \psi_0 \rangle \right| . \tag{3.11}$$

For the first test of the time evolution, the special case with $H_2 = 0$ is considered, which makes M a measure of similarity of the time evolved state with the initial state.
The Loschmidt echo is most easily computed in the eigenbasis, since it is not dependent on the basis used, and the eigenbasis is utilized for time evolution anyway. In the matrix picture:

$$\langle \psi_0 | e^{-iHt} | \psi_0 \rangle = \sum_\lambda \langle \lambda | c_\lambda^* e^{-i\lambda t} c_\lambda | \lambda \rangle = \sum_\lambda c_\lambda^*(0) c_\lambda(t) = \mathbf{c}^*(0) \cdot \mathbf{c}(t). \tag{3.12}$$

For the expectation values of observables, the state vector has to be transformed back into the natural basis because access to the natural spin states is needed in order to evaluate the action of the operators. For example, measurement of $\langle S_i^z \rangle$ is done as follows: For the state vector $\mathbf{c}$ in the natural basis, every state represented by each component like in eq. (3.8) is iterated over and the spin state ($\hat{=}$ bit) of the i'th component of the integer s_a is read out. The expectation value is then

$$\langle S_i^z \rangle_t = \sum_{a,b} c_a^*(t) \, \langle a | S_i^z | b \rangle \, c_a(t) = \sum_a |c_a(t)|^2 S_i^z, \tag{3.13}$$

since the operator S_i^z is diagonal in the natural basis. Analogously, the spin-spin correlation operator $S_i^z S_{i+n}^z$ is handled.

3.2. Tests of the time evolution

We would like to check, whether our time evolution as computed in the previous chapter gives the right results. For this reason, different tests are carried out and compared to theoretical predictions for certain special cases of the dynamics.

3.2.1. Short-time evolution

The goal is to check, whether the computed time evolution is correct up to a small time t. We start from the Heisenberg equation of motion

$$\frac{\mathrm{d}O_H}{\mathrm{d}t} = i[H, O_H], \tag{3.14}$$

where H is the Hamiltonian and

$$O_H(t) = e^{(iHt)} O e^{(-iHt)}. \tag{3.15}$$

The subscript H is dropped in what follows. Using the Baker-Campbell-Hausdorff formula $\mathrm{Ad}_{\exp iHt} = \exp \mathrm{ad}_{iHt}$ and expanding to second order, we get

$$O(t) \approx O(0) + i[H, O]t - \frac{1}{2}\,[H, [H, O]]\, t^2. \tag{3.16}$$

We want to consider the expectation value of the ith spin $\langle S_i^z \rangle$ for the total antiferromagnetic state

$$|a\rangle = |\uparrow\downarrow\uparrow\downarrow \ldots \downarrow\uparrow\rangle\,. \tag{3.17}$$

As the Heisenberg equation also holds for expectation values of operators, our expansion reads

$$\langle S_i^z \rangle_t = \langle S_i^z \rangle_0 + i\,\langle [H, S_i^z] \rangle\, t - \frac{1}{2}\,\langle [H, [H, S_i^z]] \rangle\, t^2 + \mathcal{O}(t^3). \tag{3.18}$$

From eq. (3.4) it is apparent that the linear term drops out, since all angular momentum eigenstates with different S^z are orthogonal to each other. Following the same line of reasoning, and using $S^{\pm}S^{\mp} = \mathbf{S}^2 - (S^z)^2 \pm S^z$, one can see that

$$\begin{aligned}
\langle\psi|\,[[S_i^z, H], H]\,|\psi\rangle &= \langle\psi|\,\left[(S_{i-1}^+ S_{i-1}^- + S_{i+1}^+ S_{i+1}^-)S_i^z - S_i^+ S_i^- S_{i-1}^z - S_i^+ S_i^- S_{i+1}^z\right]|\psi\rangle \\
&= \langle\psi|\,\Big[\left(\mathbf{S}_{i-1}^2 - (S_{i-1}^z)^2 + S_{i-1}^z + \mathbf{S}_{i+1}^2 - (S_{i+1}^z)^2 + S_{i+1}^z\right) S_i^z \\
&\qquad - \left(\mathbf{S}_i^2 - (S_i^z)^2 + S_i^z\right)\left(S_{i-1}^z + S_{i+1}^z\right)\Big]\,|\psi\rangle\,.
\end{aligned} \tag{3.19}$$

Evaluating this expression for the state given in eq. (3.17) results in the following approximation for the short-time evolution:

$$\langle S_i^z \rangle_t = \pm\frac{1}{2} \mp \frac{1}{2}t^2 + \mathcal{O}(t^3), \tag{3.20}$$

where the upper signs are to be used with a spin up as the initial i state ($|\ldots \underbrace{\uparrow}_{i} \ldots\rangle$) and vice versa. In fig. 3.1, the time evolution of $\langle S_1^z \rangle$ computed with the program is plotted for variable system sizes $N = 4, 6, 8, 10, 12, 14$ with $\mu = 0$, $\lambda = 0$ in eq. (3.2). The dashed blue line is the short-time approximation eq. (3.20), which correctly describes the short-time behaviour of the system. Furthermore, it can be shown that for an infinite system size, the expectation value of the spin can be expressed using the zeroth Bessel function [citation needed!]:

$$\langle S_i^z \rangle_t \Big|_{N\to\infty} = \mp\frac{1}{2} J_0(2t), \tag{3.21}$$

which is also shown in fig. 3.1. As N increases, the expectation value computed by the program matches this theoretical prediction longer and longer. Overall, this is a clear indication that the time evolution our program delivers is correct.

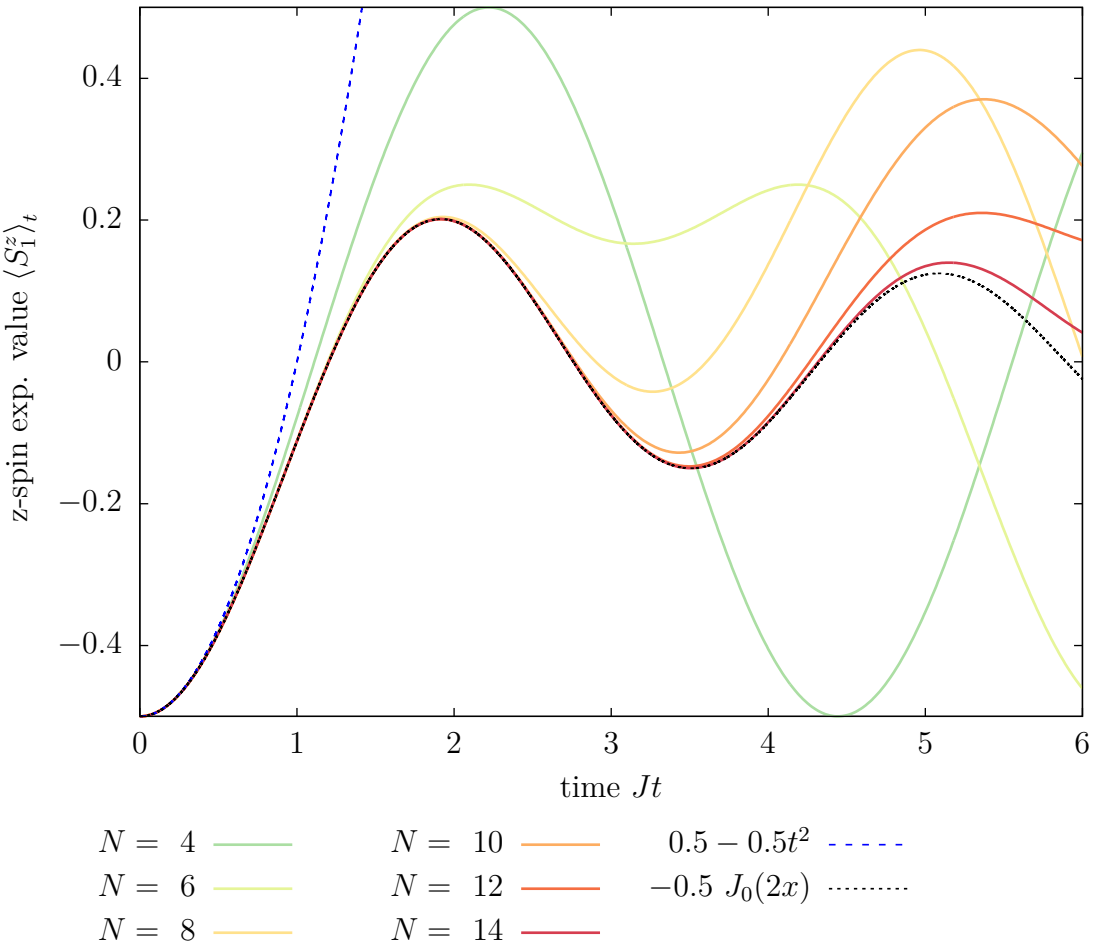

Figure 3.1.: In color: Short-time evolution of the expectation value for the first spin of the total antiferromagnetic state eq. (3.17) for different N. In blue-dashed: Short-time approximation calculated by means of a Baker Campbell Hausdorff-expansion. In black-dashed: Theoretical calculation for an infinite-sized system.

4. Ergebnisse

Test. . . citation: [4] F5 - Test:

$$\langle \Psi | \, | \Phi \rangle \tag{4.1}$$

in eq. (4.1) wird. . . $\langle 8|s|7|6\rangle$

Griechische Buchstaben:

$$\alpha\beta\chi\delta\varepsilon\varphi\gamma\eta\iota\kappa\lambda\mu\nu\pi\theta\rho\sigma\tau\upsilon\varsigma\xi\psi\zeta \tag{4.2}$$

$$\Delta\Phi\Gamma\Lambda\Xi\Psi\Sigma\Upsilon\Omega \tag{4.3}$$

$$\langle \Psi | \hat{H} | \Psi \rangle \tag{4.4}$$

$$\tag{4.5}$$

$$\boldsymbol{V} = \vec{V} \tag{4.6}$$

$$\tag{4.7}$$

Label eqs. (4.3) and (4.5)

$(\partial_\mu \partial^\mu + m^2)\Psi = 0$

$\frac{5}{8} = z$

$A \circ B$

$A \equiv B$

$$\backslash \bigcap \times \wedge \bigcap \bigcup \subset \supset \leq \geq \dot{A}\ddot{B}\sqrt{A} \Big| \int_{-\infty}^{\infty} \mathrm{d}x$$

$$\partial_\mu F^{\mu\nu} = \mu_0 j^\nu \tag{4.8}$$

$$\partial_\mu \tilde{F}^{\mu\nu} = 0 \tag{4.9}$$

5. Diskussion

Text...

5.1. Unterkapitel

Text...

5.1.1. Unterkapitel

Text...

6. Zusammenfassung

Text...

A. Calculation of $[S_i^z, H] = 0$

B. zweiter Anhang

Text...

Bibliography

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Danksagung

Dank...

Erklärung nach §13(8) der Prüfungsordnung für den Bachelor-Studiengang Physik und den Master-Studiengang Physik an der Universität Göttingen:

Hiermit erkläre ich, dass ich diese Abschlussarbeit selbständig verfasst habe, keine anderen als die angegebenen Quellen und Hilfsmittel benutzt habe und alle Stellen, die wörtlich oder sinngemäß aus veröffentlichten Schriften entnommen wurden, als solche kenntlich gemacht habe.
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Göttingen, den May 23, 2016

(Eric Bertok)