NeNa

Untertitel

Projektarbeit

im Fachbereich Physik

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Zusammenfassung

Zugsamenfassung: Ziel, Methoden, Ergebnisse, Schlussfolgerungen

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Listings

Abkürzungsverzeichnis

API	Application Programming Interface
LAMMPS	Large-scale Atomic/Molecular Massively Parallel Simulator

Symbolverzeichnis

Symbol	Bedeutung	Einheit
B	magnetische Flussdichte	T
D	Elektrische Flussdichte	$\mathrm{A\,s\,m^{-2}}$

1 Einleitung

Einleitung: Wieso sollte diese Arbeit gelesen werden?

2 Aufgabenstellung

We are here trying to calculate optical absorbtion spectra with vasp. The atomic configuration is a cavity inside a neon crystal that was proposed to be filled with either a single sodium atom or two sodiumm atoms (a sodium dimer). Now the first step was to find configurations of cavities, i.e. how many neon atoms will be replaced by an inserted sodium atom and subsequntly by a sodium dimer. This substitution number will be denoted as S in the following thesis. For these specific configurations the optical absorbtion spectra will be calculated and compared with the experiment.

3 Theory

3.1 Statistical Mechanics

First we consider the system of the crystal of Neon Atoms as a canonical ensemble, this means it will be described under the assumption of an infinitely large heat bath by Boltzmann statistics. The probability distribution of members of the ensemble will then be

$$p(\vec{\mathbf{q}}, \vec{\mathbf{p}}) = \frac{e^{-\beta H(\vec{\mathbf{q}},\vec{\mathbf{p}})}}{\int \cdots \int e^{-\beta H(\vec{\mathbf{q}},\vec{\mathbf{p}})} \mathrm{d}^{3N}\vec{\mathbf{q}} \mathrm{d}^{3N}\vec{\mathbf{p}}}, \tag{3.1}$$

with N being the number of particles.

Now an ensemble is to be understood as many fictional copies of the same system representing the states that a system will explore when propagating in time according to Hamilton's equation of motion. The ensemble distribution represents the relative number of times that an ergodic system will come by a given state after an infinite amount of time has passed. Now for a crystal in principle this still holds. At low temperatures though the phase space that is being explored can be abstracted in such cases. The reason is that the system will for a given finite time usually explore only nearby points in the phase space. This is the crystal configuration but allowing for dynamics such as lattice vibrations and thermal movement of the atoms with respect to their lattice site. So for a given initial point in phase space the system will mostly explore its proximity until it probabilistically jumps to another volume of phase space whose proximity then will be explored for some further time. Now this means the systems lattice configuration has changed which at low but non zero temperature should be reasonable. We now consider these volumes of phase space (being approximately confined regions, i.e. configurations of e.g. a crystalline structure) to be discrete states that the system can be in. So our canonical distribution now is a discrete one, each state representing such a configuration volume. What's left is to figure out what state of the still continuously possible states inside will be used to represent each configuration. We in this work will use the state $(\vec{\mathbf{q}}_{0i}, \vec{\mathbf{p}}_{0i})$ that locally minimizes $H(\vec{\mathbf{q}}, \vec{\mathbf{p}})$. Such a minimum can be found by employing a relaxation calculation in Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS). The Boltzmann distribution now follows to be:

$$p(\vec{\mathbf{q}}_{0i}, \vec{\mathbf{p}}_{0i}) = \frac{e^{-\beta H(\vec{\mathbf{q}}_{0i},\vec{\mathbf{p}}_{0i})}}{\sum_n e^{-\beta H(\vec{\mathbf{q}}_{0n},\vec{\mathbf{p}}_{0n})}}. \tag{3.2}$$

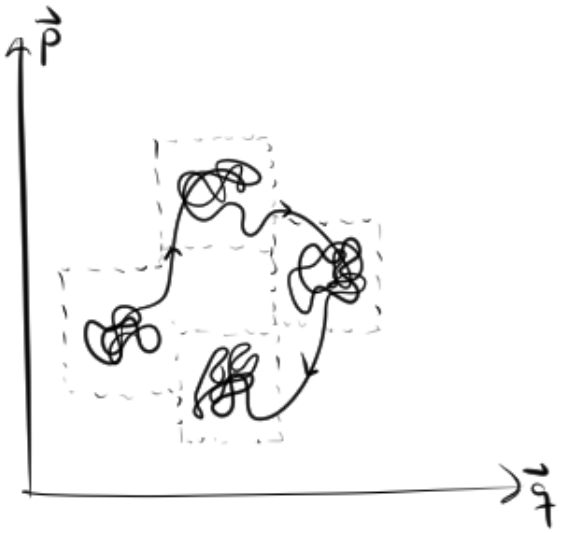

Figure 3.1: configurations volumes in phase space

grand canonical ensemble with two chemical components

sub term of grand canonical ensemble with only ne1 and ne2

3.2 Relaxation in LAMMPS

relaxation theory form lammps described in Bitzek, Koskinen, Gahler, Moseler, Gumbsch, Phys Rev Lett, 97, 170201 (2006)

3.3 Simulated Annealing

The object that is being annealed is a state vector containing binary information for every lattice site. It refers to the ideal static lattice of the neon structure. A positive value or 1 refers to an atom being present in the initial structure and a negative value or 0 means the neon atom is vacant at this site. So every digit of the binary state refers to a certain specific lattice site. The energy functional of the annealing process will be the energy after minimization (i.e. relaxation) of the above described state vector. This state vector therefore refers to an initial pre-relaxation configuration where sites are simply removed with LAMMPS.

Listing 3.1: Simulated annealing algorithm

```
stateVector = [1,1,1,1,1,1,1,1,1,1,1,1,1,1,1,1]

for i in N:
  alpha = (Tend / Tstart) ** (1 / N)
  T = Tstart * (alpha**i)


  n = randomInt(1,len(stateVector))
  stateVector[n] = 1 - stateVector[n]

  stateVectorOld = stateVector


  EOld = minimizeEnergy(stateVectorOld)
  E = minimizeEnergy(stateVector)


  if E >= EOld:
    stateVector = stateVectorOld
  elif random(0,1)<=exp(-1/T*(E-EOld)):
    stateVector = stateVectorNew
```

3.4 Symmetry optimization

In the case of a single sodium atom inserted in the neon crystalline structure the configurations of removed neon atoms the highly symmetrical structure was exploited to reduce redundant minimization calls in the annealing routine, by identifying symmetrically equivalent structures and caching them. By applying rotation and reflection matrices of the octahedral symmetry group to a single configuration, all equivalent configurations can quickly be created. By sorting them lexicographically and picking e.g. the first, one ensures every redundant set of configurations is always represented by the same configuration.

Hopefully explanation for cohesive energy

4 Erstes Kapitel

4.1 Einrichten dieser Vorlage

→ Füge in der main.tex alle relevanten Metainformationen wie Titel, Autor, ... usw. ein.

→ Ersetze das Logo in *Inhalt/Bilder/logo.png* mit dem passenden Logo und passe ggf. den Dateinamen und -endung in *Sonstiges/Titelblatt.tex* an

→ Passe den Anhang in *Verzeichnisse/Anhang.tex* entsprechend an.

4.2 Drucken

In der *main.tex*:

- oneside in twoside ändern
- openright einkommentieren
- Den Befehl \myemptypage hinter dem Titelblatt einkommentieren

In *Config/Packages.tex*:

- alle farblichen links im hyperref package auskommentiern

In *Config/Seitenstil.tex*:

- pagemark von \cfoot{} in \ofoot{} tauschen

4.3 Text

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Donec aliquam lorem feugiat nibh dapibus, at blandit erat pretium. Aliquam erat volutpat. Quisque tempus dui at augue aliquet mattis. Aliquam erat volutpat.

4.4 Bilder

Bilder in dem Ordner *Inhalt/Bilder* hinterlegen.

Figure 4.1: Placeholder Image

4.5 Programmcode

Programmcode in dem Ordner *Inhalt/Code* hinterlegen.

Listing 4.1: Code Placeholder

```
1 print("hello world!")
```

4.6 Tabellen

Zum einfacheren erstellen von Tabellen

Table 4.1: Placeholder table

Spalte 1	Spalte 2
a	1
b	2
c	3

4.7 Zitieren

Hier ein einfaches Zitat [**bibkey**].

Bibliographie Einträge in *Verzeichnisse/Literatur.bib* hinterlegen.

4.8 Abkürzung

Abkürzungen in dem Ordner *Verzeichnisse/Abkürzungsverzeichniss.tex* hintelegen.

Beim ersten Verwenden wird die Abkürzung ausgeschrieben, beim zweiten mal wird nur die Abkürzung benutzt.

Erste Verwendung: Application Programming Interface (API)
Zweite Verwendeung: API

4.9 Aufzählungen

Normale Aufzählung:

- Stichpunkt 1
- Stichpunkt 2
- Stichpunkt 3

Aufzählung mit custom Symbolen:

xyz Stichpunkt 1

abc Stichpunkt 2

! Stichpunkt 3

4.10 Referenzieren

Eine Referenz zu unserem Bild 4.1
Eine Referenz zu unserer Tabelle 4.1
Eine Referenz zu der Section Bilder 4.4

4.11 Textstyle

Kursiver Text
Bold Text
`Mono Spaced Text` (Für bsp. Programmcode)

4.12 Formeln

Referenz für Mathematik in Latex

$$\Gamma_I = \sigma\left(W_I\left[h_t|X_t\right]\right) \quad \text{(Input Gate)} \tag{4.1}$$

$$\Gamma_O = \sigma\left(W_O\left[h_t|X_t\right]\right) \quad \text{(Output Gate)} \tag{4.2}$$

$$\Gamma_F = \sigma\left(W_F\left[h_t|X_t\right]\right) \quad \text{(Forget Gate)} \tag{4.3}$$

Symbolbeschreibungen werden in dem Symbolverzeichniss unter *Verzeichnisse/Symbolverzeichniss.tex* hinterlegt.

So werden Formeln im Text angegeben x^2 und so kann man im Text einen übersichtlicheren Bruch verwenden $^{kg\,m}/_{s^2}$.

4.13 Sections

4.13.1 subsection

subsubsection

5 Zweites Kapitel

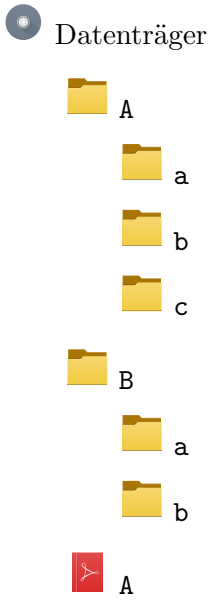
Zweites Kapitel

6 Ausblick

Ausblick

A Anhang

A.1 Inhalt des beigefügten Datenträgers



Eidesstattliche Erklärung

Ich, Gabriel Sommer, versichere hiermit, dass ich die vorliegende Arbeit selbstständig verfasst und keine anderen als die angegebenen Quellen und Hilfsmittel benutzt habe, wobei ich alle wörtlichen und sinngemäßen Zitate als solche gekennzeichnet habe.

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Wien, den July 15, 2025

Gabriel Sommer