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Investigation of a new representation of spin

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Degree project C in physics 15 hp

July 2023

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Abstract

The Bose-Hubbard Model, a tight binding model within solid state theory can be solved exactly using a number theoretical approach. From this approach, in the two sited Bose-Hubbard model, the hopping term in the model takes the form of a Pauli x matrix. The hopping term can be interpreted as a two energy level system or a dimer with k+1 particles. The statistical properties of this dimer is investigated assuming Boltzmann distribution. The partition function and particle density on each site in the dimer is calculated for spin 1/2 system. The entropy and average energy is also calculated. The particle density is calculated and plotted as a function of temperature for the spin 1/2,1,3/2 and 2 system. At low temperature the particles are more likely to be found in the lower energy site and at high temperatures the particles is equally distributed at the both sites.

Sammanfattning

Bose-Hubbard modellen är en tight binding modell inom fasta tillståndets fysik som kan lösas exakt genom att använda en talteoretisk lösningsmetod. Genom att göra detta med bara två interagerande platser i modellen tar hoppingtermen i modellen formen av en Pauli x-matris. Hopping modellen kan tolkas som ett system med två energinivåer eller en så kallad dimer med k+1 partiklar. Dimerens statistiska egenskaper undersöks utifrån Boltzmannfördelningen. Partitionsfunktionen och partikeldensiteten på varje plats i dimeren beräkn- as för ett spin 1/2 system, tillsammans med entropin och medelenergin. Vidare är partikeldensiteten beräknad och plottad som funktion av temperaturen för spinn 1/2, 1, 3/2 och 2 system. Vid låg temperatur befinner sig partiklarna i dimeren i den lägre energinivån och vid hög temperatur är partiklarna jämt fördelade i de två energinivåerna.

Contents

1   Introduction

The world consists of many different materials that are consistently being used in new technology. Research to create new materials with properties that are relevant for this are constantly being done. The theoretical research provide an understanding of the properties of materials through models. Materials are made of atoms in different structures corresponding to interactions between the atoms. Modelling the materials these interactions can be taken into consideration in many ways leading to numerous models.

This study aims to investigate the relation between spin-systems and a two-particle boson system. The Bose-Hubbard model, a tight binding model within solid state theory can be solved exactly using prime factorization. The two sited hopping term then takes the form of a Pauli x-matrix. This can be seen as a representation of spin as a two energy level system, that will be called a dimer. This interpretation of spin as a dimer is investigated through the statistical properties of the dimer using the concepts of quantum mechanics and statistical mechanics. For this a proper introduction to these topics will be continued in the following section, followed by the model and method that has be used. Thereafter the calculations are presented and finally this will be discussed.

2   Theoretical background

2.1   Quantum mechanics and Dirac formalism

This project is based on the fundamental concepts of quantum mechanics. In quantum mechanics, a physical system is described in a complex vector space. For continuous variables such as position and momentum of a particle this space is called Hilbert space. Each physical state is represented by a state vector which in Dirac formalism is called a ket, and the state α is written $|\alpha\rangle$. Each state have a dual correspondence, called a bra that is written $\langle\alpha|$. The bra vectors lives in a space that is dual to the ket space. Observables $\hat{O}$ are represented as linear operators in quantum mechanics, and are typically written, when acting on a state $|\alpha\rangle$,

$$\hat{O}|\alpha\rangle. \tag{2.1}$$

A measurement in quantum mechanics corresponds to an operator $\hat{O}$ acting on a state $|\alpha\rangle$ [1].

2.1.1 The Hamiltonian

Energy is an important quantity in physics in general. The operator representing the total energy of a system in quantum mechanics is the Hamiltonian which is generally written as,

$$\hat{H} = \hat{T} + \hat{V}. \tag{2.2}$$

Here $\hat{T}$ is the kinetic energy and $\hat{V}$ is the potential energy of the system.

2.1.2 The quantum harmonic oscillator

One of the most important systems in physics is the simple harmonic oscillator. In quantum mechanics the system is described with the Hamiltonian,

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{mw^2 \hat{x}^2}{2}. \tag{2.3}$$

The solutions to this Hamiltonian are discrete and infinitely many, the eigenvalues and eigenstates of the systems can be found introducing ladder operators, also known as creation and annihilation operators. By applying the operator one simply go up or down on the ladder or in other words increase and decrease the energy. These operators are not Hermitian and are written,

$$\hat{a} = \sqrt{\frac{m\omega}{2\hbar}} \left(\hat{x} + \frac{i\hat{p}}{m\omega} \right), \tag{2.4}$$

$$\hat{a}^\dagger = \sqrt{\frac{m\omega}{2\hbar}} \left(\hat{x} - \frac{i\hat{p}}{m\omega} \right), \tag{2.5}$$

the annihilation and creation operator respectively. The commutator is

$$[\hat{a}, \hat{a}^\dagger] = 1. \tag{2.6}$$

The number operator can be defined from this as,

$$\hat{N} = \hat{a}^\dagger \hat{a}. \tag{2.7}$$

From this the Hamiltonian can be rewritten in terms of the number operator,

$$\hat{H} = \hbar\omega(\hat{N} + \frac{1}{2}). \tag{2.8}$$

Equation (2.8) is a useful since $\hat{H}$ and $\hat{N}$ commute and therefore can be diagonalized simultaneously. The eigenvalues of the number operator $\hat{N}$ are defined as:

$$\hat{N}\,|n\rangle = n\,|n\rangle\,, \tag{2.9}$$

where $|n\rangle$ is the eigenvectors of the number operator. The eigenvalues of the Hamiltonian in this basis can then be written as:

$$\hat{H}\,|n\rangle = (n + \frac{1}{2})\hbar\omega\,|n\rangle\,. \tag{2.10}$$

So the energy eigenvalues of the Hamiltonian are equidistant,

$$E_n = (n + \frac{1}{2})\hbar\omega. \tag{2.11}$$

In the eigenbasis the annihilation and creation operator will add and erase one quanta from the total energy and will affect the state according to the following equations,

$$\hat{a}\,|n\rangle = \sqrt{n}\,|n-1\rangle\,, \tag{2.12}$$
$$\hat{a}^\dagger\,|n\rangle = \sqrt{n+1}\,|n+1\rangle\,. \tag{2.13}$$

Since $n \geq 0$ a lowest state can be defined. The eigenvector $|0\rangle$ is called the ground state or vacuum state and corresponds to the minimum energy of the system $E_0 = \frac{\hbar\omega}{2}$ (one quanta) [1].

2.1.3 Second quantization

Consider a many particle system. The particles in the system can have different energies and are indistinguishable. Using quantum mechanics formalism the system can be described with a state vector,

$$|n_1, n_2, ..., n_i, ...\rangle\,, \tag{2.14}$$

where n_i is the number of particles in each subsystem, corresponding to a specific energy. This state vector is part of the vector space called Fock space. The ground state of all vectors in Fock space is when there are no particles at all, the vacuum state,

$$|0, 0, 0, ..., 0\rangle \equiv \left|\vec{0}\right\rangle\,. \tag{2.15}$$

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Similarly as for the one particle case, annihilation and creation operators are used to change the number of particles in each state, such that,

$$\hat{a}_i^\dagger \ket{n_1, n_2, ..., n_i, ...} = \ket{n_1, n_2, ..., n_i + 1, ...}, \quad (2.16)$$

$$\hat{a}_i \ket{n_1, n_2, ..., n_i, ...} = \ket{n_1, n_2, ..., n_i - 1, ...}. \quad (2.17)$$

The number operator is defined as the sum of the particles at each state and the occupation number operator is defined as $\hat{n}_i = \hat{a}_i^\dagger \hat{a}_i$.

$$\hat{N} = \sum_{i=0}^{i} \hat{n}_i = \sum_{i=0}^{i} \hat{a}_i^\dagger \hat{a}_i. \quad (2.18)$$

The commutation relations of the annihilation and creation operators are different depending on if the wave function is symmetric or antisymmetric. The operators are called bosonic and fermionic operators respectively, since bosons have symmetric wave functions and therefore can be in the same state, but the antisymmetric fermions obey the Pauli exclusion principle, only two fermions with different spins can be in the same state. In table 1 the conditions for the bosonic and fermionic operators are presented [1].

Bosons	Fermions
$[\hat{a}_i^\dagger, \hat{a}_j^\dagger] = 0$	$\{\hat{a}_i^\dagger, \hat{a}_j^\dagger\} = 0$
$[\hat{a}_i, \hat{a}_j] = 0$	$\{\hat{a}_i, \hat{a}_j\} = 0$
$[\hat{a}_i^\dagger, \hat{a}_j] = \delta_{i,j}$	$\{\hat{a}_i^\dagger, \hat{a}_j\} = \delta_{i,j}$

Table 1: Commutation relations for bosons and fermions in second quantization. The notation for the commutator is $[A, B] = AB - BA$ and the anti commutator $\{A, B\} = AB + BA$.

2.1.4 Representation of spin in quantum mechanics

Spin is an intrinsic property that is used to characterize particles. Particles can have integer and half integer spin. The half integer spin particles are called fermions and the integer spin particles are called bosons. For a spin $1/2$ system the spin components can be obtained using the 2×2 Pauli matrices,

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \quad (2.19)$$

Spin 1/2 is then defined as $S_i = \frac{\hbar}{2}\sigma_i$. For spin 1, 3/2, 2.. the corresponding matrices are square matrices of higher dimensions, $3 \times 3, 4 \times 4$ and so on [1].

2.2 Statistical mechanics

Statistical physics describes the physical properties of macroscopic systems. Macroscopic systems consists of a large number of particles, that can be atoms or molecules. In statistical mechanics an important distinction can be made between microscopic states and macroscopic states. The microscopic state defines the state on a atomic scale while the macroscopic state can be described by a few observable quantities on the macroscopic level. For each macroscopic state there are several microscopic states and the total system can therefore be described such that each macroscopic state with a number of microscopic states. From this relation one can form the quantity statistical weight which describes all possible outcomes and can be written as,

$$\Omega(E, V, N, \alpha). \tag{2.20}$$

The energy E varies within a small interval $E + \delta E$, the volume V and the particle number N are specifying the macroscopic state and α contains additional variables. The statistical weight, also called thermodynamic probability is a measure of the number of microscopic states for a given macroscopic state. A system with N particles that can be in two possible state can have 2^N possible microscopic states for a given macroscopic state and thus the statistical weight for the macroscopic state is

$$\Omega(n) = \binom{N}{n} = \frac{N!}{n!(N-n)!}. \tag{2.21}$$

For an isolated system in equilibrium, two postulates can be defined,

- For an isolated system all microscopic states have the same probability to occur (for given E, V and N).

- The system is in equilibrium for the α that maximizes the statistical weight $\Omega(E, V, N, \alpha)$.

For an isolated system, the entropy can be introduced as a measure of disorder of the system

$$S(E, V, N, \alpha) = k \ln \Omega(E, V, N, \alpha), \tag{2.22}$$

k is the Boltzmann constant. Entropy is an important quantity since it relates the macroscopic observed quantity to the microscopic properties of the system [2].

2.2.1 Boltzmann distribution: The partition function

For a system in equilibrium in a heat bath with temperature T the Boltzmann distribution can be used. The probability for a system to be in a particular state is given by the Boltzmann distribution,

$$p_r = \frac{1}{Z} e^{-\beta E_r}, \tag{2.23}$$

with the normalization factor Z that is also called the partition function,

$$Z = \sum_r e^{-\beta E_r}. \tag{2.24}$$

E_r is the energy of the system, $\beta = \frac{1}{kT}$ where T is the temperature and k is the Boltzmann constant. The partition function is the sum of all microscopic states of the system. From the partition function, the average energy can be calculated as

$$\langle E \rangle = -\frac{\partial Z}{\partial \beta}. \tag{2.25}$$

The entropy of the system is defined as,

$$S = \frac{\partial}{\partial T}(kT \ln Z) = -k \ln Z + \frac{1}{T}\langle E \rangle. \tag{2.26}$$

This is a more useful way to define entropy, then the earlier notation that was introduced in equation (2.22) [2].

2.3 Solid state theory

Solid state theory describes the interactions of atoms in lattices that form solids. In a solid the atoms don't move freely and are typically bound at certain distances from each other which is useful when doing models.

2.3.1 Statistical mechanics in Solid state theory

A solid consists of many particles so the system can not be prepared in a well defined quantum state but since a solid can be described by its macroscopic state the thermal expectation value can be specified from the temperature T, volume V and particle number N. The thermal expectation value in a solid $\hat{A}$ can thus be written as,

$$< \hat{A} >= \frac{1}{I} \sum_{i=0}^{I} \langle i| A |i \rangle .$$ (2.27)

The thermal expectation value is defined by the microscopic states $|i\rangle$, $i = 1, 2, ..., I$ of the solid for fixed T, V, N. By inserting the completeness relation $\sum_i |i\rangle \langle i| = \hat{1}$, and the trace notation $\text{Tr}(A) = \sum_n \langle n| A |n\rangle$, one can rewrite the expression,

$$< \hat{A} >= \sum_n \langle n| \left(\frac{1}{I} \sum_{i=0}^{I} |i\rangle \langle i| \right) \hat{A} |n \rangle ,$$ (2.28)

which is equivalent to

$$< \hat{A} >= \text{Tr}\left(\hat{\rho}\hat{A} \right),$$ (2.29)

where $\hat{\rho}$ is the statistical operator or density operator

$$\hat{\rho} = \frac{1}{I} \sum_{i=0}^{I} |i\rangle \langle i| .$$ (2.30)

The statistical operator describes all the possible outcomes of the system, gives the distribution of the system. Connecting back to section 2.2 where statistical mechanics was explained, the statistical operator is a distribution function that depends on the system. For a solid that can be described with thermodynamic variables, the Boltzmann distribution can be used. The canonical ensemble can be extended to the grand canonical ensemble for a fixed temperature T and and particle number N is,

$$\hat{\rho}_G = \frac{1}{Z_G} e^{-\beta(\hat{H}-\mu\hat{N})},$$ (2.31)

where μ is the chemical potential, $\hat{N}$ is the number operator, $\hat{H}$ is the Hamiltonian of the system. The constant $\beta = \frac{1}{kT}$ where k is the Boltzmann constant. The grand partition function Z_G is,

$$Z_G = \text{Tr}\left(e^{-\beta(\hat{H} - \mu\hat{N})}\right). \tag{2.32}$$

The grand canonical ensemble is useful for a system that has both a heat bath T and a particle reservoir N [3].

2.3.2 The Bose-Hubbard model

The Bose-Hubbard model can be used to describe interactions in a solid and includes nearest neighbour interactions. It can be described with the Hamiltonian,

$$\hat{H} = \sum_n^\infty \frac{U}{2}\hat{N}_n(\hat{N}_n - 1) - \mu\hat{N}_n - t(\hat{a}_n^\dagger\hat{a}_{n+1} + \hat{a}_{n+1}^\dagger\hat{a}_n). \tag{2.33}$$

U is the Coloumb potential, μ is the chemical potential and t is the hopping parameter. The last term of equation (2.33) is the so called hopping term and describes the interaction between two neighbouring atoms. The state vectors can be rearranged in terms of prime numbers $p_1....p_k$,

$$|n\rangle = |p_1\rangle \odot |p_2\rangle \odot .. |p_k\rangle. \tag{2.34}$$

The symmetric tensor product $\odot$ is invariant under permutations so for example,

$$|2\rangle \odot |3\rangle \equiv |3\rangle \odot |2\rangle. \tag{2.35}$$

Figure 1: New indexing of the bosons, using prime numbers.

This is a number theoretical approach, since any integer is fully factorized in terms of prime numbers. The numbers can be written as

$$n = \prod_{p \in P} p^{a_p(n)}. \tag{2.36}$$

Factorizing the states into prime numbers and collecting the multiplicity of the prime numbers in the exponent $a_p(n)$ the annihilation and creation operators can then be defined, acting on the basis δ_n,

$$\hat{a}_p \delta_n = \sqrt{a_p(n)} \delta_{\frac{n}{p}}, \tag{2.37}$$

$$\hat{a}_p^\dagger \delta_n = \sqrt{a_p(n) + 1} \delta_{np}. \tag{2.38}$$

The basis vectors $\delta_n \to |n\rangle$ are only nonzero for the quotient $\frac{n}{p}$ that is an integer, that are the prime numbers p_k that factorizes n. To illustrate this, take the number 10 that can be decomposed into the prime numbers 2 and 5. Acting on the basis δ_{10} with the annihilation operator $\hat{a}_2$ the basis reduces to

$$\hat{a}_2 \delta_{10} = \delta_{\frac{10}{2}} = \delta_5, \tag{2.39}$$

and similarly acting on δ_{10} with $\hat{a}_5$ gives δ_2. However acting with for example $\hat{a}_3$,

$$\hat{a}_3 \delta_{10} = \delta_{\frac{10}{3}} = 0, \tag{2.40}$$

since 10 cannot be factorized by the prime number 3. Another example is the number 9 that can be factorized by the prime number 3. The multiplicity is $a_3(9) = 2$ and acting with the annihilation operator results in $\sqrt{2}\delta_3$. Using this number theoretical approach the Hamiltonian can be reformulated as,

$$\hat{H} = \sum_{n=1}^{\infty} \frac{U}{2} \hat{N}_{p_n}(\hat{N}_{p_n} - 1) - \mu \hat{N}_{p_n} - t(\hat{a}_{p_n}^\dagger \hat{a}_{p_{n+1}} + \hat{a}_{p_{n+1}}^\dagger \hat{a}_{p_n}). \tag{2.41}$$

The Hamiltonian matrix can then be calculated exactly [4].

3 Method

The two-site Bose-Hubbard model only include the nearest neighbour inter-action and the hopping term of the hamiltonian is then written,

$$\hat{H} = \hat{a}_2^\dagger \hat{a}_3 + \hat{a}_3^\dagger \hat{a}_2. \tag{3.1}$$

Here, $p_1 = 2$ and $p_2 = 3$ are prime numbers. Using the number theoretic model the Hamiltonian can be exactly calculated in a k-particle subspace represented by a $(k+1) \times (k+1)$ tridiagonal matrix,

$$\hat{H}|_{\mathbb{H}^{\odot k}} = \begin{pmatrix} 0 & \sqrt{k} & & & & \\ \sqrt{k} & 0 & \sqrt{2(k-1)} & & & \\ & \sqrt{2(k-1)} & 0 & \sqrt{3(k-2)} & & \\ & & \sqrt{3(k-2)} & 0 & & \\ & & & & \ddots & \\ & & & & & \sqrt{k} \\ & & & & \sqrt{k} & 0 \end{pmatrix}, \tag{3.2}$$

for k = 0,1,2,3,... . The Hamiltonian is spanned by the vectors, $\mathbb{H}^{\odot k} = \text{span}\{\delta_{2^\alpha 3^{k-\alpha}} : \alpha = 0, 1, 2, ..., k\}$. The Hamiltonian is invariant in each k-particle subspace, meaning that $[\hat{H}, \hat{N}] = 0$. The matrix elements are equivalently written as,

$$\hat{H}|_{\mathbb{H}^{\odot k}} = \sum_{\alpha=0}^{k} \sqrt{(k-\alpha)(\alpha+1)}\delta_{2^{\alpha+1}3^{k-\alpha-1}} + \sqrt{\alpha(k-\alpha+1)}\delta_{2^{\alpha-1}3^{k-\alpha+1}}. \tag{3.3}$$

To examplify this, for k=1 the matrix becomes,

$$\hat{H}|_{\mathbb{H}^{\odot 1}} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \tag{3.4}$$

k=2:

$$\hat{H}|_{\mathbb{H}^{\odot 2}} = \begin{pmatrix} 0 & \sqrt{2} & 0 \\ \sqrt{2} & 0 & \sqrt{2} \\ 0 & \sqrt{2} & 0 \end{pmatrix}, \tag{3.5}$$

and k= 3:

$$\hat{H}|_{\mathbb{H}^{\odot 3}} = \begin{pmatrix} 0 & \sqrt{3} & 0 & 0 \\ \sqrt{3} & 0 & 2 & 0 \\ 0 & 2 & 0 & \sqrt{3} \\ 0 & 0 & \sqrt{3} & 0. \end{pmatrix}. \tag{3.6}$$

While Equation (3.4) can be recognised as the Pauli x-matrix σ_x describing spin 1/2, Equation (3.5) and (3.6) similarly corresponds to spin 1 and spin 3/2. More generally the solutions to the Hamiltonian in a k-particle subspace corresponds to k/2 spin in x-direction. The Pauli matrices σ_i are an essential part of the formulation of spin, where that spin directions are represented as $S_i = \frac{\hbar}{2}\sigma_i$, for $i = x, y, z$ [5].

3.1 Representation as particles in the dimer

The k-particle subsystem connects increasing integer and half integer spin via it's matrix form to k+1 particles in the hopping term, interpreting this as a system of two energy levels with k+1 particles to form a so called dimer consisting of two energy levels, 2 and 3,

$$\begin{matrix} 3 \\ 2 \end{matrix} \begin{pmatrix} \cdot \\ \cdot \end{pmatrix}. \tag{3.7}$$

For example, k=1 represents a two particle system such that that the dimer can take three different forms,

$$\begin{matrix} 3 \\ 2 \end{matrix} \begin{pmatrix} \bullet\bullet \\ {} \end{pmatrix}, \begin{pmatrix} \bullet \\ \bullet \end{pmatrix}, \begin{pmatrix} {} \\ \bullet\bullet \end{pmatrix}.$$

For k=2 there are 3 particles in the system and the dimer can have four different forms,

$$\begin{matrix} 3 \\ 2 \end{matrix} \begin{pmatrix} \bullet\,\bullet\,\bullet \\ {} \end{pmatrix}, \begin{pmatrix} \bullet\bullet \\ \bullet \end{pmatrix}, \begin{pmatrix} \bullet \\ \bullet\bullet \end{pmatrix}, \begin{pmatrix} {} \\ \bullet\,\bullet\,\bullet \end{pmatrix},$$

and so on. Note that the particles to be bosons, meaning they can be in the same state. The dimer as a representation of spin will now be investigated from its statistical behavior. Since the hopping term is an atomic interaction within solid state theory the distribution function of the dimer will be assumed to follow the Boltzmann distribution.

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4 Calculations

Using the method described in [5] the spin y-matrix takes the form,

$$\hat{H}_y = i\hat{a}_2^\dagger \hat{a}_3 - i\hat{a}_3^\dagger \hat{a}_2. \tag{4.1}$$

And for the z-matrix the Hamiltonian

$$\hat{H}_z = -\hat{a}_2^\dagger \hat{a}_2 + \hat{a}_3^\dagger \hat{a}_3. \tag{4.2}$$

The latter is on diagonal form and for simplicity in the calculations this will be used but corresponds to the same distribution as for the original hopping term. Using the number representation the partition function can be calculated according to equation (2.32). For bosons the chemical potential is zero, since the number of particles at a given state is not restricted. The hopping parameter has until now been ignored but are now used in the calculation of the partition function.

4.1 Spin 1/2 system

For spin 1/2 the dimer contains two particles. Using the definition of the number operator according to equation (2.18) the grand partition function can be written as,

$$Z_G = \text{Tr}\{e^{-\beta \hat{H}}\} = \text{Tr}\{e^{-\beta(-\hat{a}_2^\dagger \hat{a}_2 + \hat{a}_3^\dagger \hat{a}_3)}\} = \text{Tr}\{e^{\beta(\hat{n}_2 - \hat{n}_3)}\}. \tag{4.3}$$

The number of microscopic states (microstates) that the system can be in is restricted by the number of particles in the system. The occupation number operators can take the values $\hat{n}_i = 1, 2, 3$ for $i = 2, 3$ but are restricted since the total particle number is $\hat{n}_2 + \hat{n}_3 = 2$ such that,

$$\hat{n}_2 = \begin{cases} 2 \longleftrightarrow 0 \\ 1 \longleftrightarrow 2 \\ 0 \longleftrightarrow 3 \end{cases} = \hat{n}_3 \tag{4.4}$$

The corresponding microstates are thus given by the difference $\hat{n}_2 - \hat{n}_3$ shown in Table 2.
The grand partition function for the spin 1/2 case is

$$Z_G = \sum_i e^{\epsilon_i} = e^{2t\beta} + e^{0 \cdot t \cdot \beta} + e^{-2 \cdot t\beta} = e^{2t\beta} + 1 + e^{-2 \cdot t\beta} = 2\cosh(2t\beta) + 1. \tag{4.5}$$

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Table 2: Microstates ϵ_i for $i = 1, 2, 3$ for spin $1/2$ system.

ϵ_1	ϵ_2	ϵ_3
2	0	-2

Using equation (2.31) the particle density at each site in the dimer can now be calculated as,

$$\langle n_i \rangle = \frac{1}{Z_G} \text{Tr}\left\{ \hat{n}_i e^{-t\beta \hat{H}} \right\}. \tag{4.6}$$

For $\hat{n}_i = 1, 2, 3$ corresponds to the microstates such that,

$$\langle n_2 \rangle = \frac{1}{Z_G}(0 \cdot e^{-2t\beta} + 1 \cdot 1 + 2 \cdot e^{2t\beta}) = \frac{1 + 2e^{2t\beta}}{2\cosh(2t\beta)}. \tag{4.7}$$

And similarly ,

$$\langle n_3 \rangle = \frac{1}{Z_G}(2 \cdot e^{-2t\beta} + 1 \cdot 1 + 0 \cdot e^{2t\beta}) = \frac{1 + 2e^{-2t\beta}}{2\cosh(2t\beta)}. \tag{4.8}$$

In Figure 2 the density distribution is plotted as a function of T for respective site.
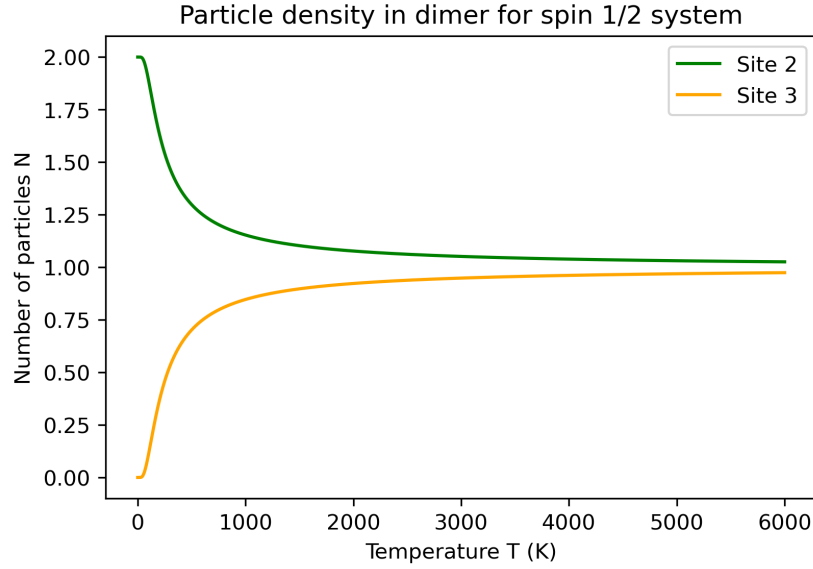

Figure 2: Particle density in site 2 and 3 of the dimer is plotted as a function of the temperature T for a spin $1/2$ system.

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Furthermore, the average energy and the entropy of the system is calculated according to equation (2.25) and (2.26).

$$\langle E \rangle = -\frac{\partial \ln}{\partial \beta}(e^{2t\beta} + 1 + e^{-2t\beta}) = -\frac{4t \sinh{(2t\beta)}}{2\cosh{(2t\beta)} + 1}, \qquad (4.9)$$

and the entropy,

$$S = k \ln Z_G + \frac{1}{T}\langle E \rangle = k \ln(\cosh{(2t\beta)} + 1) - \frac{1}{T}\frac{4t \sinh(2t\beta)}{2\cosh{(2t\beta)} + 1}. \qquad (4.10)$$

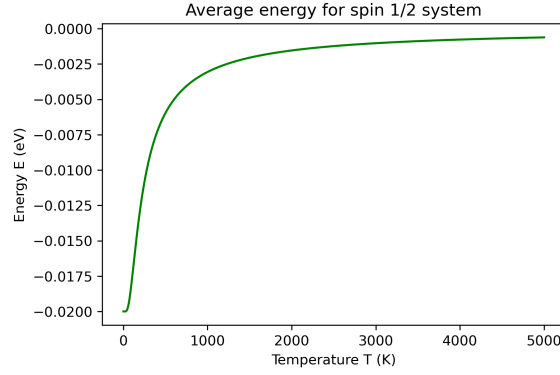The average energy and the entropy is plotted in Figure 3 and 4 respectively.

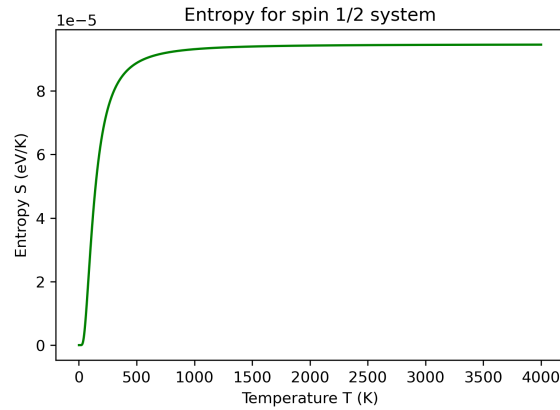Figure 3: The average energy E as a function of the temperature T.

Figure 4: Entropy E for the system as a function of the temperature T.

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4.2 Spin 1 system

For the spin 1 system, there are 4 microstates with the corresponding energies shown in table 3.

Table 3: Microstates ϵ_i $i = 1, 2, 3, 4$ for spin 1 system.

ϵ_1	ϵ_2	ϵ_3	ϵ_4
3	1	-1	-3

The partition function for the spin 1-system is

$$Z_G = e^{-3t\beta} + e^{-t\beta} + e^{t\beta} + e^{3t\beta} = 2\cosh\left(\beta t\right) + 2\cosh\left(3\beta t\right). \qquad (4.11)$$

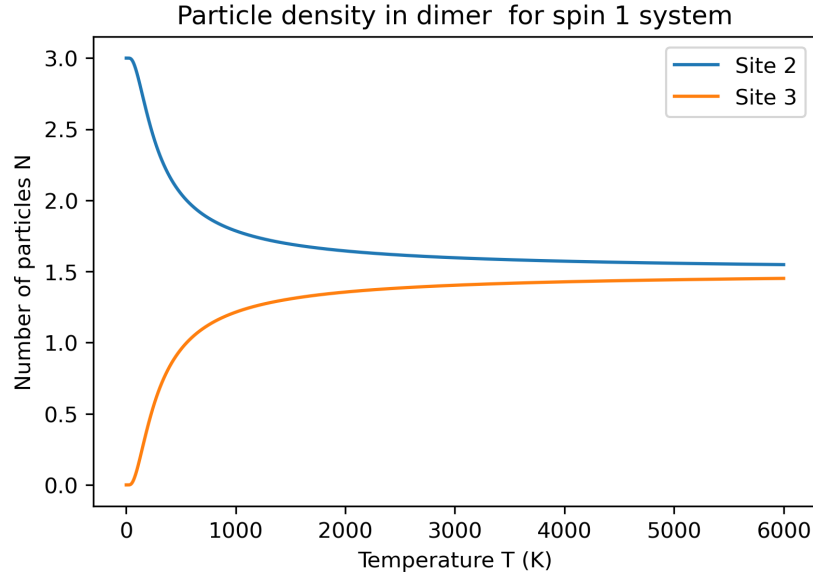The particle densities in the dimer are plotted in Figure 5.

Figure 5: Particle density in site 2 and 3 of the dimer is plotted as a function of the temperature T for a spin 1 system.

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4.3 Higher order spin

For higher spin the number of microstates increases with the number of particles in the system. In Figure 6 the particle densities for spin 1/2, spin 1, spin 3/2 and spin 2 are normalized and plotted together.
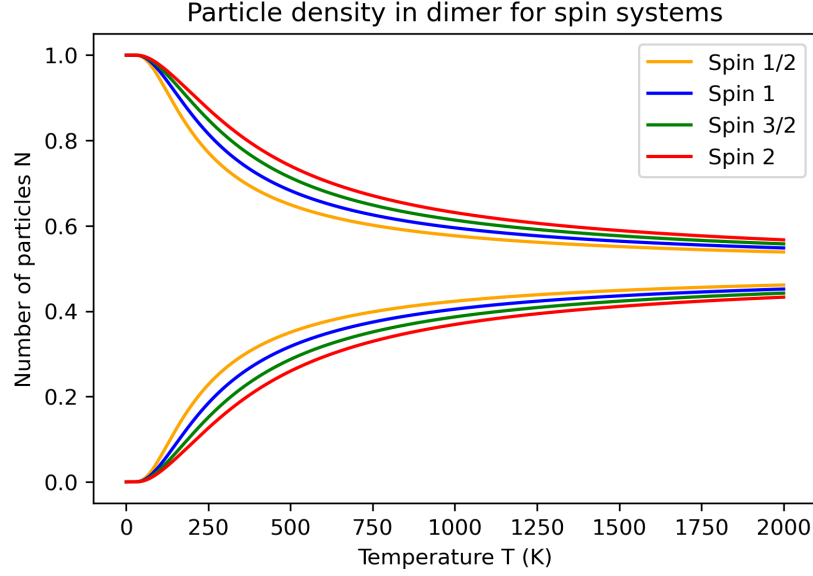

Figure 6: The normalized particle densities with both site for the spin 1/2, spin 1, spin 3/2 and spin 2 systems.

5 Discussion

In this thesis the representation of spin as a dimer has been investigated, using statistical mechanics as it is a solid state theoretical model. Using the Boltzmann distribution the particle distributions for the spin 1/2, spin 1 systems are plotted in Figure 2 and 5. According to the plots, the particles are more likely to be in the lower energy state at low temperature T and goes towards an equal distribution between the two sites at high temperature T, going towards a more disordered state which from a physical point of view seems reasonable. In Figure 6 of the normalized distributions for different spin the graphs becomes flatter for higher spin. Since the number of particles in the system increase, and so the number of microstates, this can be thought

of as it being more difficulty to move several particles between the sites, then one, thus it requires more energy. The average energy and entropy for the spin 1/2 system is plotted in Figure 3 and 4. The energy are negative at low temperature and goes towards zero has the temperature increases. This can be explained by the form of the Hamiltonian $\hat{H}_z$ in Equation 4.2 seeing at is is written as the difference in particles at site 3 and 2. The energy on site 2 is defined as negative, thus the maximum energy when both particles are on this site corresponds to negative energy. The entropy is increasing with the temperature, and the systems goes towards being more disordered so this is reasonable from a physical point of view.

It is important to discuss the assumptions that has been made on this theoretical model. The formulation of the dimer is based on the number theoretical approach that the Bose-Hubbard was originally solved for. The particles in this subsystem are assumed bosons (they can be on the same site). Using the Boltzmann distribution can seem arbitrary and might not be the correct way to look at the system. Modelling spin with bosonic operators are not a new thing. For example Schwinger's Oscillator model of angular momentum [1] is similar however the visualization is different. The interpretation in this model is a two spin 1/2 particles corresponding to spin up and down. This is distinctly different from a two-level system in which we can have infinite many particles corresponding to different spin.

From a societal and ethical point of view, one can argue if it is worth to spend money in theoretical research instead of applications of this or in other part of the society. All research can be used in a harmful and unethical way if it's in the wrong person's hand.

5.1   Conclusion

An important part of theoretical work is the visualization by models. Describing the concepts of physics and finding connection between the different parts is a way to understand the concepts better. Describing spin as a 2 energy level system is interesting and could be investigated further. It would be interesting to use the dimer model and apply it on spin chains for example. A comparison with other distribution functions would also be interesting.

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