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MAGNETIC AND THERMODYNAMIC PROPERTIES OF QUANTUM SPIN NANOSTRUCTURES

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Abstract

The magnetic and thermodynamic properties can predicted from the solution of the Ising model applied to spin arrays. Two-dimensional spin lattices are commonly solved by Monte Carlo simulation, in the literature. This work aims to solve 3D spin arrays along nanostructures, such as nanotubes.

Key-words: Spin; Nanotubes; Ising model; Metropolis; Monte Carlo.

Introduction

The Ising Model is a mathematical model that doesn't correspond to an actual physical system. However, it's extremely helpful to have an actual system in mind, so that we can refer to something explicit and build physical intuition. The model consists of discrete variables that represent magnetic dipole moments of atomic "spins", in a lattice of sites, that can be in one of two states -1 and $+1$ [4].

In this work we evaluate magnetic and thermodynamic properties of metallic nanostructures, such as nanotubes, through the solution of the Ising model via Monte Carlo simulations.

Models and properties

Consider a set Γ of lattice sites, each with a set of adjacent sites forming a d-dimensional lattice. For each lattice site $k \in \Gamma$ there is a discrete variable σ_k such that $\sigma_k \in +1, -1$, representing the spin of the site. A spin configuration, $\sigma = (\sigma_k)_{k\in\Gamma}$ is an assignment of spin value to each lattice site. For any two adjacent sites $i, j \in \Gamma$ there is an interaction J_{ij}. Also a site $j \in \Gamma$ has an external magnetic field h_j interacting with it. The energy of a configuration σ is given by the Hamiltonian function [5]

$$H(\sigma) = -\sum_{\langle ij\rangle} J_{ij}\sigma_i\sigma_j - \mu\sum_j h_j\sigma_j, \tag{1}$$

where the first sum is over pairs of adjacent spins (every pair is counted once). The notation $\langle ij\rangle$ indicates that sites i and j are nearest neighbors. The magnetic moment is given by μ. Note that the sign in the second term of the Hamiltonian above should actually be positive because the electron's magnetic moment is antiparallel to its spin, but the negative term is used conventionally. Tow atoms heterogeneous spin systems (Figure 1) are will be studied here by a mixed spin-3/2 (Fe) and spin-1/2 (Al), using the Ising-model.

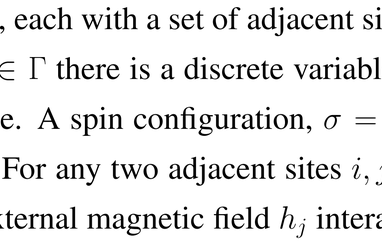

Figure 1: Tow atoms heterogeneous spin system representation.

In this case the Hamiltonian used is

$$H = -J\sum_{\langle i,j\rangle} S_i\sigma_j - J_\sigma\sum_{\langle i,j\rangle}\sigma_i\sigma_j - J_S\sum_{\langle i,j\rangle} S_iS_j - K_v\left(\sum_i S_i^2 + \sum_j \sigma_j^2\right) \tag{2}$$

Monte Carlo simulation

Since every spin site has ± 1 spin, there are 2^L different states that are possible. This motivates the reason for the Ising model to be simulated using Monte Carlo methods [**?**]. We will treat the above Hamiltonian (eq. 1) by employing Monte Carlo simulations.

The Metropolis algorithm used Monte Carlo integration to simulate random selections from a probability density function (Figure 2). To determine whether or not equilibrium has been reached, the overall energy of the system is tracked and when the rate of energy change slows down significantly, we can say that the system is approximately at equilibrium.

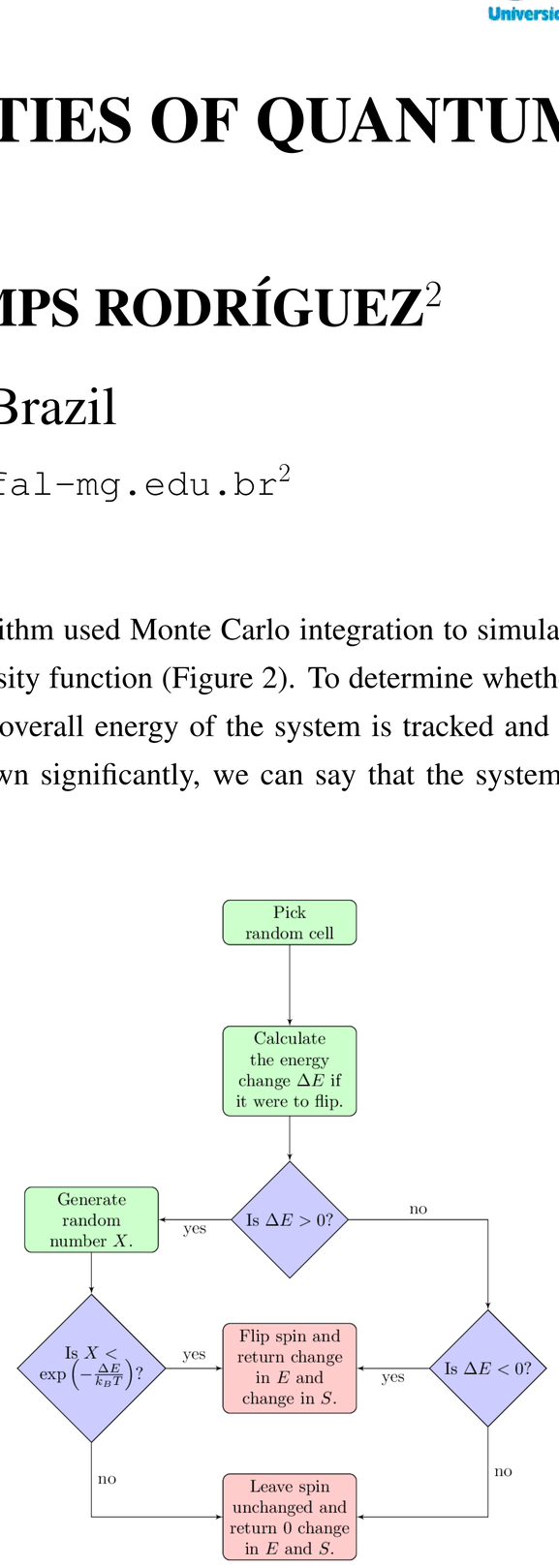

Figure 2: Metropolis algorithm flowchart.
Source: Adapted from [1].

Once this state has been reached, the Metropolis algorithm is run for another 10,000 and the measurements of E and S are taken from this and later used to calculate the magnetic and thermodynamic properties.

To improve the efficiency of the algorithm, the total energy is only calculated once at the start of the simulation. For every subsequent iteration, the energy would be updated by adding or subtracting energy change caused by flipping (or not flipping) a site [1].

All the computing will be done in R language - R version 4.1.2 - as well as R will be used for graphing the results [2]. The pseudorandom numbers generator will be the SF Mersenne-Twister algorithm [3], already implemented in R, in the function `runif()`.

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