Bulk properties of semiconductors

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Analytical and numerical calculations of the magnetic properties of a system of disordered spins in the Ising model

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Abstract. We consider a system of randomly distributed magnetic atoms and describe the exchange interaction in the Ising model with a hydrogen-like dependence of the exchange energy on distance. The density of states for such system was calculated using an advanced numerical algorithm. Furthermore, the density of states was calculated analytically. We established that finding the density of states allows calculating the dependence of magnetic susceptibility of the system on temperature and magnetic field.

Keywords: Ising model, Wang-Landau algorithm, magnetic susceptibility

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Аналитический и численный расчеты магнитных свойств системы неупорядоченных спинов в модели Изинга

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Аннотация. Мы рассматриваем систему случайно распределенных магнитных атомов в модели Изинга с водородоподобной зависимостью обменной энергии от расстояния. Плотность состояний для такой системы посчитана численно и аналитически. Показано, что, зная плотность состояний, несложно рассчитать зависимость магнитной восприимчивости системы от температуры и магнитного поля.

Ключевые слова: модель Изинга, алгоритм Ванга-Ландау, магнитная восприимчивость

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Introduction

The exchange interaction of impurity atoms in semiconductors is actively studied. Interest in this topic grew significantly after the discovery of ferromagnetism in GaAs uniformly doped with a Mn magnetic impurity [1] (not due to Mn or MnAs clusters). At the moment, active experimental studies of the magnetic properties of semiconductors doped with non-magnetic impurities are being carried out [2–4]. The distribution of impurity atoms in semiconductors is random. However, the magnetic properties of materials are primarily theoretically studied in lattices that are either regular or close to regular. The magnetic properties of systems with a completely random distribution of magnetic atoms have not been thoroughly studied. This may be due both to the complexity of the considered model and to different approaches to describing regular and irregular systems. One of the main theoretical results in this field is the work [5], which predicts the absence of long-range magnetic order in a system of randomly distributed impurities with antiferromagnetic interaction. In our previous works [6, 7], we used a more correct expression for the dependence of the exchange energy on the distance. In the hydrogen-like model, the exchange energy of two spins at a distance r can be expressed as [8, 9]:

$$J = J_0 \left(\frac{r}{a} \right)^{2.5} \exp\left(-\frac{2r}{a} \right). \quad (1)$$

It was found in [6] that magnetic ordering is possible in a system of randomly distributed magnetic impurities. As the impurity concentration increases, the so-called spin-fluctuation phase transition occurs. In this case the amplitude of fluctuation of the magnetic moment increase, while the average magnetic moment of the system is equal to zero on both sides of the phase transition.

The magnetic properties of a system of randomly distributed impurities are often calculated using numerical methods, in particular, the Metropolis-Hastings algorithm [7, 10]. This algorithm starts with a random state of the spin system which is then thermalized to the required temperature. At low temperatures, the number of steps required for thermalization increases exponentially. In addition, the system may get in a pseudoground state, separated from lower energy states by a high energy barrier. In other words, at low temperatures the system is in the spin glass phase. Therefore, the Metropolis-Hastings algorithm is not efficient at low temperatures. In the present work, we used the Wang-Landau algorithm for accurate numerical calculation of the density of states and proposed an analytical expression for the density of states for a system of randomly distributed spins.

Numerical calculation

In this paper, we consider a system of randomly distributed spins and numerically and analytically calculate the dependence of the density of states on the total exchange energy E and the magnetic moment of the system M. For convenience, we denote the average magnetic moment of one spin, normalized to unity, by m. Then the total magnetic moment of the system $M = \mu mN$. Here μ is the magnetic moment modulus of one spin, N is the total number of spins in the system. Knowing the density of states $g(E, m)$, it is easy to calculate the average magnetic moment and magnetic susceptibility of the system as a function of temperature and magnetic field.

In the Ising model each spin can be directed up or down. That is, each spin has only two possible states. However, the number of possible states for a system of N spins is 2^N. For example, the number of different states for a system of only 100 spins is more than 10^{30}, and it is impossible to enumerate all the states even with the help of the fastest computers. The density of states can be found by the random walk method [10]. However, this method is only effective near the maximum of the density of states, producing large noise at the tails. A variation of the random walk method known as the Wang-Landau algorithm [11, 12] was used in this study.

Below we briefly consider the main idea of the Wang-Landau algorithm. Energy and magnetic moment are divided into small intervals. Initially, it is considered that the density of states for all values of energy and magnetic moment is equal to 1. Then random walks start, at each step

the density of states in the corresponding interval is increased by f times, where f is the so-called modification factor. Initially, modification factor is taken equal to e, this value is chosen for convenience. Then the modification factor is gradually reduced to increase the accuracy of the calculations. In addition to the density of states, we will count how many times the system appears in each interval during a random walk and save the corresponding value in the histogram $h(E, m)$.

At each step, we randomly select one spin and try to flip it. We calculate the energy E_1 and the magnetic moment m_1 before the spin flip, and the energy E_2 and the magnetic moment m_2 after the spin flip. The flip is accepted with probability $p(1 \to 2) = \min\left(\frac{g(E_1, m_1)}{g(E_2, m_2)}, 1\right)$. That is, we always accept transitions to less probable states, and the probability of transition to a more probable state depends on the ratio of densities of state in the initial and final states. Thus, the Wang-Landau algorithm is non-Markovian chain, the probability of transition to the next state depends on the history of previous transitions.

At the moment when the histogram $h(E, m)$ is flat enough, that is, the maximum and minimum values differ by no more than some specified amount (usually 80–90%), we decrease the modification factor and reset the histogram to zero. The algorithm terminates when the modification factor becomes small enough, so the density of states is known quite accurately.

Fig. 1 shows the calculated density of states for a system of $N = 512$ spins. The size of the system was chosen based on a reasonable calculation time. For example, it took about a week to calculate the density of states shown in the figure. The color in the figure shows the decimal logarithm of the density of states, that is, the maximum and minimum value of the density of states differ in this figure by 130 orders of magnitude. Notice that the noise on the tails of the density of states is minimal.

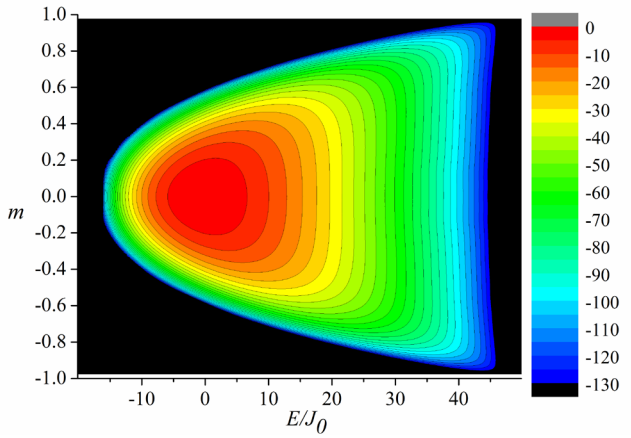

Fig. 1. Decimal logarithm of the density of states $g(E, m)$, normalized to the maximum value. Calculation for a system of $N = 512$ spins and concentration $na^3 = 0.03$

The complexity of the problem can be reduced and the size of the system can be increased if the density of states is calculated for a fixed value of the magnetic moment. The algorithm differs only in that at each step we try to simultaneously flip two randomly selected, oppositely directed spins in order to preserve the total magnetic moment of the system. Performing the numerical calculation, we generated a configuration of $N = 8192$ spins and then calculated the density of states for various values of the magnetic moment of the system for the same configuration of spins in space. The calculations were performed on the supercomputer at Peter the Great St. Petersburg Polytechnic University, allowing to calculate the density of states in parallel for 25 different values of the magnetic moment. The size of the system was determined based on a reasonable computation time, provided that the required computational accuracy is achieved.

It should be noted that the value of the energy of the system at the maximum of the density of states depends on the spatial distribution of the spins. This dependence is purely statistical in nature, the relative dispersion of the average energy decreases as $1/\sqrt{N}$ with an increase in the total number of particles in the system. However, the spread was still significant with the available size of the system. For this reason, we did not average over different spatial configurations.

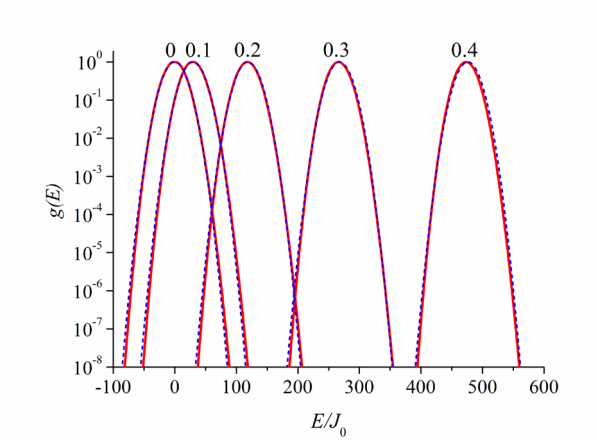

Fig. 2. Densities of states depending on the energy for different values of the magnetic moment m, the values are signed near the corresponding curves. Red lines correspond to numerical calculations using the Wang-Landau algorithm, blue dashed line to theoretical calculation by Eq. (5)
Calculations were performed for a system of $N = 8192$ spins and concentration $na^3 = 0.05$

The results of numerical calculations show that, at a fixed value of the magnetic moment, the density of states has a form close to a normal distribution (Fig. 2). Fig. 3 shows the position of the maximum and the dispersion of the distribution depending on the magnetic moment of the system m. It can be concluded that, in the considered range, the dispersion remains practically constant, and the position of the maximum has a quadratic dependence on m.

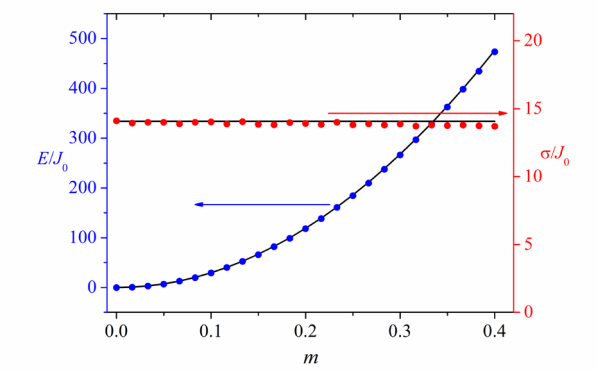

Fig. 3. Comparison of the average energy and dispersion of the distribution versus magnetic moment of the system, obtained by numerical simulation (dots) and by analytical equations (lines). The calculations were carried out for a system of $N = 8192$ spins and a concentration $na^3 = 0.05$

Analytical model

The density of states $g(E, m)$ can also be calculated analytically. The total exchange energy of the system of N interacting spins is the sum of $N(N-1)/2$ pair energies, each of which is a random variable. In accordance with the central limit theorem, the distribution of such a sum should be close to normal. This explains the form of the density of states obtained by numerical calculation. In order to write an analytical expression for the density of states, it is necessary to calculate the mean value and dispersion of the total exchange energy E. To calculate the average exchange energy, we first consider the system of spins with one orientation. We denote the average energy of the exchange interaction of one spin with all others as $\overline{J_1}$. The following expression [6] can be obtained for the exchange energy (1):

$$\overline{J_1} = \sqrt{\frac{\pi}{2}}\frac{945\pi}{2^8} na^3 J_0. \qquad (2)$$

Then, in a system of p "up" spins and q "down" spins, the average exchange energy is

$$\overline{E} = \frac{1}{2}\left(p\left(\frac{p-q}{p+q}\right) + q\left(\frac{q-p}{p+q}\right)\right)\overline{J_1} = \frac{1}{2}Nm^2\overline{J_1}. \quad (3)$$

For a system of randomly oriented spins, the average exchange energy of one spin is zero and the dispersion of the exchange energy of one spin will be equal to $\overline{J_1^2}$. Then the dispersion of the total exchange energy will be equal to $\sigma^2 = \frac{1}{2}N\overline{J_1^2}$. For the exchange energy (1), one can obtain

$$\sigma^2 = \frac{7!\pi}{2^{15}}na^3NJ_0^2 = \frac{315\pi}{2^{11}}na^3NJ_0^2. \quad (4)$$

According to the results of numerical simulation, the dispersion of the exchange energy of the system is practically independent of m for $|m| < 0.4$. For large m, this is not the case; in particular, a fully magnetized system ($m = \pm 1$) has only one state, which means that the dispersion is zero. Therefore, the theoretical formulas written below are not applicable in the ferromagnetic phase at low temperatures.

Finally, in the Ising model, the total number of states in a system of N spins is 2^N, and the number of states with exactly p "up" spins is $C_N^p = C_N^{\frac{N(m+1)}{2}}$. Thus the density of states can be expressed as

$$g(E,m) = C_N^{\frac{N(m+1)}{2}}\frac{1}{\sqrt{2\pi\sigma}}\exp\left(-\frac{\left(E-\overline{E}\right)^2}{2\sigma^2}\right) = C_N^{\frac{N(m+1)}{2}}\frac{1}{\sqrt{2\pi\sigma}}\exp\left(-\frac{\left(E-\frac{1}{2}Nm^2\overline{J_1}\right)^2}{2\sigma^2}\right). \quad (5)$$

Let us assume that the density of states $g(E, m)$ is known from numerical or analytical calculations. In a magnetic field, the energy of the system will be the sum of the exchange energy E and the energy of interaction with the magnetic field $MB = \mu NmB$. Then the probability density versus energy E and magnetic moment m will be described by the Gibbs distribution and will be proportional to $g(E,m)\cdot\exp\left(-\frac{E+\mu NmB}{kT}\right)$. Using this expression, we can calculate all the parameters of the system of spins, such as the average magnetic moment or magnetic susceptibility:

$$\overline{M} = \frac{\mu N}{Z}\int dE\sum_m mg(E,m)\exp\left(-\frac{E+\mu NmB}{kT}\right), \quad (6)$$

where Z is statistical weight.

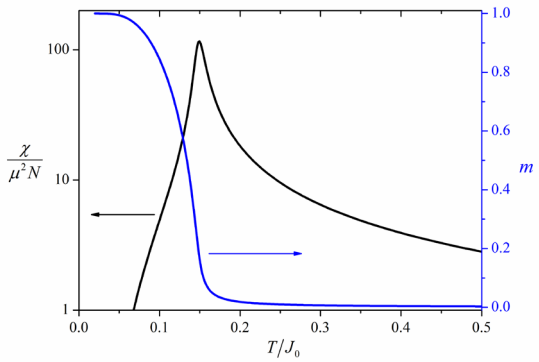

Fig. 4. Dependence of magnetic susceptibility and average magnetic moment per one spin on temperature

The main difficulty of analytical calculations in such a model is the calculation of binomial coefficients for large numbers. For example, for the studied system of 8192 spins, their value reaches 10^{2463}. However, the modern programming language julia supports both work with numbers of arbitrary length and parallel calculations, makes it possible to perform calculations in a reasonable time. As an example, Fig. 4 shows the calculated temperature dependence of magnetic susceptibility and average magnetic moment in a weak magnetic field.

Conclusion

To summarize, in this paper, we describe an efficient algorithm for numerical calculation of the density of states in a system of randomly distributed spins. Furthermore, we propose an analytical method for calculating the density of states in such a system. It is shown that knowing the density of states of the system allows to easily find the thermodynamic parameters of the system, in particular, the dependence of magnetic susceptibility and magnetic moment on temperature.

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