Semiclassical Approximation for the Curie – Weiss Model

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Abstract. The paper is devoted to the construction of spectral series and the estimation of the approximation accuracy for the operator of the Curie – Weiss model. In the course of work, the operator is reduced to a tridiagonal form in the subspace of the original space, then to a second-order difference equation. The admissibility of reducing an operator to a subspace is presented. It is shown that the difference equation can be considered in the discrete semiclassical approximation. In the obtained classical system, the dependence of the turning points on the model parameters is investigated. The asymptotics of the spectrum of the Curie-Weiss operator is calculated and the accuracy of the approximation is estimated.

1. Introduction
The paper investigates the quantum Curie – Weiss model, which is the quantum Ising model considered in the mean field approximation.

The Ising model is a mathematical model of ferromagnetism in statistical mechanics. Let us represent the system of spins in the form of a graph, in which the set of vertices is a set of particles, and the edges are the existing connections between the spins.

In the Curie – Weiss model, the mean field approximation consists in representing the spin graph as complete, that is, it is assumed that every pair of spins are interacting. Such a model is presented, for example, in [1]. In the mentioned work, the $2^N$-dimensional Hilbert space $\mathcal{H}_N = \mathbb{C}^{2^N}$ with basis $\{e_{n_1} \otimes \cdots \otimes e_{n_N}\}_{n_1,...,n_N=1,2}$, where $e_1 = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ corresponds to the "up" spin and $e_2 = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$ - the "down" spin, $N < \infty$ is the number of spins. In the space $\mathcal{H}_N$, the operator of the system is defined as

$$\hat{H} = -\frac{1}{2N} \sum_{x,y=1}^{N} \sigma_3(x)\sigma_3(y) - B \sum_{x=1}^{N} \sigma_i(x),$$

where $B$ is the external magnetic field; $\sigma_i(x)$ is the Pauli matrix acting on the spin with the number $x$, ($i = 1, 2, 3$).

In [2] and [3], various properties of the Curie – Weiss model and its generalizations to more complex spaces are studied. In [2], the physical properties of classical models in a magnetic field and without its action are considered, and various approaches to research are presented. In [3], the analysis of phase transitions for the canonical and microcanonical ensembles is carried out in the Curie - Weiss - Potts model, which is the Potts model considered in the mean field approximation. The Potts model is a generalization of the Ising model, which considers the interaction of spins on a crystal lattice.

The Curie-Weiss model finds application in the study of the effect of quantum tunneling of the magnetization of single-molecule magnets (SMM) [4], such as Mn$_i$, Mn$_4$, and Ni$_4$ SMM.
In this paper, we study the application of the discrete semiclassical approximation (see in [5]) to the quantum Curie – Weiss model for calculating the spectrum of operator (1).

The aim of this work is to study the applicability of the Bohr – Sommerfeld quantization rule to the calculation of the spectrum of the Curie – Weiss operator. The tasks are as follows: represent operator (1) in the form of a difference equation in appropriate basis, find the turning points of the difference operator, and calculate the spectrum in the semiclassical approximation.

2. Curie–Weiss model operator as a second order difference operator
First, we reduce operator (1) to a tridiagonal form using the result of paper [1].

Theorem [1]. In the basis of the space of symmetrized tensors \( \mathcal{H}_N \), operator (1) is a tridiagonal matrix of dimension \((N + 1) \times (N + 1)\):

\[
\begin{align*}
-\frac{1}{2N} (2n_+ - N)^2 & \quad \text{main diagonal}, \\
-B\sqrt{(N - n_+)(n_+ + 1)} & \quad \text{upper diagonal}, \\
-B\sqrt{(N - n_+ + 1)n_+} & \quad \text{lower diagonal};
\end{align*}
\]

where \( n_+ \) is the number of "up" spins.

Consider the stationary Schrödinger equation of the system with operator (2)

\[
\hat{H}\psi = E\psi,
\]

where \( \psi = (\psi(0), ..., \psi(N)) \) is the wave function in the basis of symmetrized tensors.

Changing variables \( \hbar = \frac{1}{N} x = \frac{n_+}{N} \), \( E := -\frac{B}{N} y(x) = \psi(k) \); we obtain the second order Hermitian difference equation

\[
a(x + h)y(x + h) + u(x)y(x) + a(x)y(x - h) = Ey(x),
\]

with the boundary conditions \( y(-h) = y(1 + h) = 0 \).

The coefficients of equation (3) are as follows:

\[
a(x) = B \left( (1 - x + \frac{1}{N})x \right)^{1/2}, \quad u(x) = \frac{1}{2}(2x - 1)^2.
\]

3. Operator in full space
The subspace of symmetrized tensors is only a contraction of the complete space \( \mathcal{H}_N \) with a basis in the form of orthonormal linear combinations of tensors, on which operator (1) is defined.

Denote \( S_x = \sum_{i=1}^{N} \sigma_1(i), S_y = \sum_{i=1}^{N} \sigma_2(i), S_z = \sum_{i=1}^{N} \sigma_3(i) \). The operators \( S_\alpha, \alpha = x, y, z \), form the rotation group of the Lie algebra \( \text{SO}(3) \).

Consider the Casimir operator \( K = S_x^2 + S_y^2 + S_z^2 \). In the original basis \( \{e_{n_1} \otimes ... \otimes e_{n_N}\}_{n_1,...,n_N=1,2} \), the operator \( K \) is a matrix of dimension \((2^N \times 2^N)\). This matrix has \( 2^N \) eigenvalues: for \( i = 0, 1, ..., \left[ \frac{N}{2} \right] \) there is an eigenvalue \((N - 2i + 1)^2 - 1\) of multiplicity \( \binom{N}{i} \left( \frac{(N - 2i + 1)^2}{N - i + 1} \right) \). The multiplicity of the eigenvalues corresponds to the terms of the Clebsch – Gordan decomposition series when \( N \) spins of size \( \frac{N}{2} \) are combined.

Linear combinations of eigenvectors \( K \) corresponding to the same eigenvalues, with appropriately chosen coefficients, define an orthonormal basis in the space \( \mathcal{H}_N \).

With an appropriate ordering of the basis vectors, operator (1) has a block-diagonal structure. Let us denote the elements of the basis as \( \tilde{q}_{n,i,n_+} \); where \( n = N - 2k, i = 1, ..., \left( \binom{N}{k} \right) \frac{N-2k+1}{N-k+1}, n_+ = 0, 1, ..., N - 2k; \) where \( k = 0,1, ..., \left[ \frac{N}{2} \right] \).
Then operator (1) in the complete basis has the following block-diagonal form:

\[
\begin{array}{cccccc}
  k & 0 & 1 & \ldots & \frac{N}{2} \\
  n & N & N-2 & \ldots & 1, \text{if } N \text{ is odd} \\
  i & 1 & 1 & \ldots & N-1 & 1, \text{if } N \text{ is even} \\
  n_+ & 0 & 1 & \ldots & N & 0, \text{if } N \text{ is even} \\
  \end{array}
\]

For a fixed \( k \), we have \( \binom{N}{k} \) identical tridiagonal square blocks, the diagonal elements of which are specified by Theorem [1] for a system of \( N-2k \) spins with multiplication of diagonal elements by the constant \( \frac{N-2k+1}{N-k+1} \).

In the presented basis order, the index \( n \) has the meaning of the number of particles in the system; \( i \) - block number corresponding to the number \( n \); and \( n_+ \), as before, is the number of up spins.
The spectrum of operator (4) consists of combining the spectra of its blocks. Each block is an operator similar to operator (1) in the space of symmetrized tensors, with the only difference in the normalization constant for the spin interaction. However, this difference does not change the approach to calculating the spectrum of blocks, and narrowing the original space does not lead to a loss of generality.

4. Asymptotics of the spectrum of the system operator

Next, we will use the results of [5]. Consider the classical system with the Hamiltonian \( H(x, p, \hbar) \), which is the Weyl symbol of the operator of the difference equation (3)

\[
H(x, p, \hbar) = u(x) + 2a \left( x + \frac{\hbar}{2} \right) \cos p.
\]

Hamiltonian (5) is a periodic function and defines a classical mechanical system on a cylinder.

Investigating the turning points of the classical system with Hamiltonian (5) on the plane \((x, E)\), we obtain two different nondegenerate cases depending on the strength of the external magnetic field. In the limit \(N \to \infty\), the cases are as follows (Figure 1): (a) \(B \in (0, 1)\); (b) \(B \geq 1\).

![Figure 1. Turning points on the plane \((x, E)\).](image)

In case (a), we have one pair of turning points between the lower boundary of the spectral cluster (the range of energy changes) and the separatrix and two pairs of turning points between the separatrix and the upper boundary of the cluster. In case (b), we have one pair of turning points over the entire region of the spectral cluster.

The spectrum of operator (2) will be calculated for the more interesting case \(B \in (0, 1)\) using the Bohr–Sommerfeld quantization rule for difference equations [5]. In this case, the quantization rule has the form

\[
\frac{1}{2\pi} \oint_{\gamma(E)} x dp = \hbar \left( n + \frac{\sigma}{4} \right) + O(\hbar^2),
\]

where \(\gamma(E)\) – are the classical trajectories of the system; \(n \in \mathbb{Z}\); the index \(\sigma = 0\), if the trajectory \(\gamma\) goes around the cylinder, \(\sigma = 2\) otherwise. In this problem, \(\sigma = 0\) for energies above the separatrix and \(\sigma = 2\) for energies below the separatrix.

The accuracy of calculating the spectrum according to rule (6) is estimated through the absolute error \(AE(E)\) of asymptotic values with respect to the numerical values obtained by calculating the spectrum of operator (2) as a matrix of dimension \((N + 1) \times (N + 1)\).

Let us first consider the dependence of the absolute error on the value of the eigenvalue for fixed \(N, B\) (Figure 2).
Figure 2. Dependence of the absolute error on the magnitude of the eigenvalue.

We get that \( AE(E_i) \) does not exceed \( \hbar^2 = \frac{1}{N^2} \) for all values of the spectrum, except for values lying in the neighborhood of the separatrix. Here we denote \( \hbar = \frac{1}{N} \) as a dimensionless quantity.

Let us now consider the dependence of the maximum of the absolute error as the number of particles increases (Figure 3).

Figure 3. Dynamics of the maximum absolute error.
Let us apply the linear regression method to estimate the order of absolute errors. Using the power model $y = cx^d$, where $c$ and $d$ are the estimated parameters, $x$ and $y$ are independent and dependent variables respectively; we obtain the following functional dependence of the absolute errors on $\hbar$: near the separatrix $\max(AE) \approx 0.62\hbar^{2.05}$; outside the separatrix $\max(AE) \approx 0.07\hbar^{1.04}$.

Taking into account the accuracy of the regression results, we conclude that the order of the error in calculating the asymptotics of the spectrum values outside the neighborhood of the separatrix is close to $O(\hbar^2)$, and the magnitude of the error does not exceed $\hbar^2$; while an error of the order of $O(\hbar)$ is observed in the vicinity of the separatrix.

The following conclusions can be drawn from the performed numerical simulation. The Bohr-Sommerfeld quantization rule gives the correct result when calculating the asymptotics of the spectrum, including at the boundaries of spectral clusters, where, generally speaking, it has not been proven. In the vicinity of the separatrix, the quantization rule is not applicable and does not give the correct result.

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Acknowledgments
Author wishes to acknowledge assistance and encouragement from colleague Vybornyi E V. The work was supported by the project group “Asymptotic methods in problems of modeling physical processes” on MIEM NRU HSE.