Ergodicity of the extended anisotropic 1D Heisenberg model: response at low temperatures

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Abstract

We present the results of exact diagonalization calculations of the isolated and isothermal on-site static susceptibilities in the anisotropic extended Heisenberg model on a linear chain with periodic boundary conditions. Based on the ergodicity considerations we conclude that the isothermal susceptibility will diverge as \( T \to 0 \) both in finite clusters and in the bulk system in two non-ergodic regions of the phase diagram of the system.

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It is often thought that the ergodicity - the property to explore the whole Hilbert space during time evolution - is a natural attribute of a physical system and, moreover, that its possible violation is hard to observe. Ergodicity assumptions are usually made when passing through various self-consistent schemes in determining susceptibilities, correlation functions etc. Nevertheless, non-ergodic behavior may manifest under certain circumstances. The purpose of this article is to show how non ergodicity can significantly change the properties of the system and may become in principle observable.

When dealing with the static response of a quantum system two definitions of the susceptibility are usually considered: the static "isolated" or "Kubo susceptibility" \( \chi_0 \) and the isothermal one \( \chi^T \) [1]. These two definitions correspond to different environmental conditions under which the response is measured. Namely, \( \chi_0 \) is derived upon the assumption that the system is isolated, while in order to measure \( \chi^T \) one has to maintain the system in thermal equilibrium with an external bath at a given temperature. As it was pointed out by Kubo and Suzuki [2], a necessary and sufficient condition for these two response functions to coincide is the ergodicity of the system. By considering as a specific example the response function of an operator \( A \) to a perturbation coupled to \( A \) itself, the isolated Kubo susceptibility will be:

\[
\chi_0 = -i \int_0^\infty dt \langle [A(t), A(0)] \rangle
\]

while the isothermal one:

\[
\chi^T = \int_0^\beta d\lambda \langle A(-i \lambda A) - \beta \langle A \rangle^2 \rangle.
\]

Their difference, as shown in [1,2], is given by:

\[
\chi^T - \chi_0 = \beta (\Gamma - \Gamma^{\text{erg}}),
\]

where we have introduced the quantity \( \Gamma \):

\[
\Gamma = \lim_{t \to \infty} \langle A(t)A(0) \rangle
\]

and its ergodic value

\[
\Gamma^{\text{erg}} = \langle A \rangle^2.
\]

When \( \Gamma \neq \Gamma^{\text{erg}} \) the response is said to be non-ergodic and the two susceptibilities differ. In this case, non-ergodicity becomes observable as it provides a diverging contribution to \( \chi^T \) in the limit \( T \to 0 \).

In this paper we show the results for the isolated susceptibility in the extended anisotropic Heisenberg model on a linear chain of 14 sites with periodic boundary conditions. The susceptibility has been calculated using the spectrum of the system obtained by means of the exact numerical diagonalization. The Hamiltonian of the system reads as:
ond order. One can see from (8) that the Kubo susceptibility can be rewritten as:

$$\chi_0(i, i) = -i \int_0^{\infty} dt \langle [S_i^z(t), S_i^z(0)] \rangle. \quad (7)$$

Because of the translational invariance $\chi_0(i, i)$ is independent of the site $i$.

Previously [3],[4] we have already studied the question of ergodicity of the response of $S_i^z$ in the Hamiltonian (6). We have constructed a phase diagram of (6) in the plane $J' - J_z$ for both zero and finite temperatures using as large as 26 sites clusters. We have concluded that at $T = 0$ and in the bulk limit there are two non-ergodic regions and two ergodic ones (see Fig.1 in [4]). A transition zone exists at finite sizes, which probably would become a transition line in the bulk limit. At $T > 0$ the finite-size scaling indicated that the system is always ergodic.

On Fig. 1 the Kubo susceptibility is plotted as a function of temperature for the ergodic (panel a) and non-ergodic (panel b) regions from the phase diagram obtained in [4]. While at high temperatures $\chi_0(T) \sim 1/T$, as it should be after the Curie law, the most interesting behavior is concentrated at low temperatures. One can easily show that when $T \rightarrow 0$ the Kubo susceptibility can be rewritten as:

$$\chi_0(T) = \frac{2}{N} \sum_{l=1}^{N} \sum_{E_n > E_0} \frac{|\langle 0, l | S_i^z | n \rangle|^2}{E_n - E_0} + \Omega(T), \quad (8)$$

where $N$ is the number of degenerate ground states $|0, l \rangle$, $l = 1, \ldots, N$, $| n \rangle$ is the $n$–th excited eigenstate of (6) and $\Omega(T)$ goes exponentially to zero when $T \rightarrow 0$. (8) is nothing else but the result of the perturbation theory up to the second order. One can see from (8) that $\chi_0(0)$ is non-singular and in general non-zero since all the terms under the sum have the same sign. This is not the case in the phase Non-ergodic I (see the dashed and dashed-dotted lines on the Fig. 1b)) since in this phase the ground state is doubly degenerate with all spins either up or down. Such states are eigenstates of $S_i^z$ and therefore the matrix elements in (8) vanish. All the other phases have their ground states connected to the rest of the Hilbert space by $S_i^z$ so that for them $\chi_0(0) \neq 0$.

From our data for the isolated susceptibility and by using (3), we can find the temperature dependence of $\chi^T$ as well. It is clear from (3) that in both ergodic phases (Ergodic I and Ergodic II) $\chi^T(T) = \chi_0(T)$. On the contrary, the isothermal susceptibility will diverge at low $T$ as $\Gamma/T$, where $\Gamma = 1/2 + 1/6L$ for the phase Ergodic I on a cluster of $L$ sites, and $\Gamma = 1/4$ for the phase Ergodic II, independently on $L$. Based on the finite-size scaling for $\Gamma$ made in [4] these results will hold also in the thermodynamic limit.

In conclusion, we have studied the on-site static magnetic response of (6), considering both definitions of the susceptibility. While for the isolated one the non ergodicity enters implicitly through the degeneracy of the eigenvalues, the isothermal susceptibility contains an explicit term diverging at low-$T$ in the case of non-ergodic phases. In real materials, however, this divergence might not be observable due to perturbations such as dipole–dipole interactions which destroy the conservation of $z$-component of the total spin and ensure the ergodicity.

References

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