Super-stable points and cycles on double-tetrahedral chains

G. Amatuni[1], Č. Burdik[2] H. Poghosyan[3], L. Ananikyan[3] and N. Ananikian[1 3]

[1]Condensed Matter and Polymers,CANDLE SRI, Yerevan, Armenia
[2]Faculty of Nuclear Sciences and Physical Engineering, Czeck Technical University,Prague, Czeck Republic
[3]Theoretical Physics,A. Alikhanyan National Laboratory, (former Yerevan Physics Institute), Yerevan, Armenia

E-mail: gayane@asls.candle.am

Abstract. Quantum systems with antiferromagnetic spin-1 Ising and Ising-Heisenberg interactions with single-ion anisotropy on double-tetrahedral chains can exhibit unconventional classical and quantum states responsible for the anomalous behavior of magnetization curves at low temperatures. We find super-stable points and cycles for those chains when the temperature tends to zero.

1 Introduction

The subject of our study are metallic compounds, also known as chemical compounds, containing metals combined with other elements including other metals or non-metals. These chemical compounds have unique properties that make them extremely valuable for a wide range of applications, from construction materials to electronic devices and pharmaceuticals. By studying metallic compounds, we gain insights both into natural world and potential innovation, enabling the development of new technologies. As an example can be mentioned the following compounds:

homometallic magnetic complex - $[Ni3(C_4H_2O_4)_2 - (\mu_3 - OH)_2)(H_2O)_4]_n \cdot (2H_2O)_n$;

the molecular compound - $[Ni_8(\mu_3 - OH)_4(OMe)_2(O_3PR_1)_2(O_2C^tBu)_6(HO_2C^tBu)_8]$;

natural azurite (Copper Carbonate Hydroxide) - $Cu_3(CO_3)_2(OH)_2$.

Magnetic property measurements on such compounds indicate the coexistence of both antiferromagnetic and ferromagnetic interactions between the magnetic centers, ions with spin 1, which indeed suggests to investigate theoretically the magnetic properties of such compounds. A remarkable feature of these systems is their exact solutions. Exactly solvable models are of great importance in statistical physics because they provide valuable insights into various aspects of quantum phenomena. The quantum spin systems with competing interactions in an external magnetic field can be considered as a such model [**1-5**]. In the present work, we will propose and exactly solve the antiferromagnetic spin-1 system on a double-tetrahedral chain in an external magnetic field. Double-tetrahedral antiferromagnetic chains represent a fascinating class of materials in condensed matter physics and materials science. Their complex interplay of geometry, magnetism, and quantum effects makes them critical for understanding magnetic frustration and quantum behavior in low-dimensional systems. We investigate the phenomena of super-stable points and cycles within double-tetrahedral chains. It is important to note that double-tetrahedral geometry is realized for the spin system of Cu^{2+} ions in the magnetic compound $Cu_3Mo_2O_9$, known as natural azurite (Copper Carbonate Hydroxide), can be well described by using the quantum antiferromagnetic Heisenberg model on a double-tetrahedral chain. The physical properties of the Heisenberg model on a double-tetrahedral chain have been investigated using different methods [**6**]. In our study we are using the recursion relation method. The aim of that method is to cut lattice into branches and express the partition function of all lattice through the partition function of branches. This procedure will allow to derive one- or multi-dimensional mapping for branches of the partition function. After which the thermodynamic quantities of the physical system such as magnetization, magnetic susceptibility, and specific heat can be expressed through recursion relation [**7-17**]. The aim of the study is a super-stability in the above mentioned model. We propose a non-trivial connection of super-stable points and super-stable chains to Lyapunov exponents and find out that the behavior of the maximal Lyapunov exponent via the magnetic field of multi-dimensional rational mapping has a plateau and coincides with magnetization plateau.

2 The Model

We consider the spin-1 antiferromagnetic Ising-Heisenberg model on a double-tetrahedral chain (see Figure 1) in magnetic field with the Hamiltonian:

$$H_{IH} = J(S_1S_2 + S_1S_3 + S_2S_3) + J_1(S_1 + S_2 + S_3)(\mu_0 + \mu_1) + \Delta\left(S_1^2 + S_2^2 + S_3^2 + \frac{\mu_0^2 + \mu_1^2}{2}\right) - \\ - g\mu_B h\left(S_1 + S_2 + S_3 + \frac{\mu_0 + \mu_1}{2}\right), \tag{1}$$

where

$$S^x = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \quad S^y = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix}, S^z = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix} \tag{2}$$

$$S_1 = S^z \otimes I_3 \otimes I_3, \quad S_2 = I_3 \otimes S^z \otimes I_3, \quad S_3 = I_3 \otimes I_3 \otimes S^z \tag{3}$$

$$S_{1x}S_{2x} = S_x \otimes S_x \otimes I_3, \quad S_{1y}S_{2y} = S_y \otimes S_y \otimes I_3, \quad S_{1z}S_{2z} = S_z \otimes S_z \otimes I_3 \tag{4}$$

$$S_{1x}S_{3x} = S_x \otimes I_3 \otimes S_x, \quad S_{1y}S_{3y} = S_y \otimes I_3 \otimes S_y, \quad S_{1z}S_{3z} = S_z \otimes I_3 \otimes S_z \tag{5}$$

$$S_{2x}S_{3x} = I_3 \otimes S_x \otimes S_x, \quad S_{2y}S_{3y} = I_3 \otimes S_y \otimes S_y, \quad S_{2z}S_{3z} = I_3 \otimes S_z \otimes S_z \tag{6}$$

$$S_1S_2 = S_{1x}S_{2x} + S_{1y}S_{2y} + S_{1z}S_{2z}, \quad S_1S_3 = S_{1x}S_{3x} + S_{1y}S_{3y} + S_{1z}S_{3z}, \tag{7}$$

$$S_2S_3 = S_{2x}S_{3x} + S_{2y}S_{3y} + S_{2z}S_{3z} \tag{8}$$

In the Ising-Heisenberg Hamiltonian $S_{Hi}, (i = ..., -3, -2, -1, 1, 2, 3...)$ are quantum Heisenberg spins $(S_{Hi} = S_i))$, I_3 is a 3×3 identity matrix and $\mu_i, (i = ... -1, 0, 1...)$ are classical Ising spins. The parameter J accounts for the interactions between the nearest-neighbor Heisenberg spins and J_1 is the interactions parameter for nearest-neighbor Ising and Heisenberg spins, Δ is a single-ion anisotropy parameter, h is the external magnetic field.

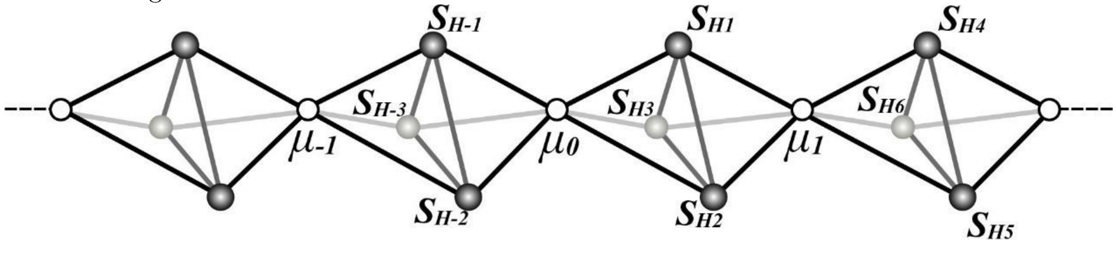

Figure 1.
The schematic of double tetrahedral chain

3 Partition Function

Consider a system made up of microstates labeled r with the energy of each microstate E_r, then the probability of the system being in a state r is given by p_r such that

$$p_r = \frac{1}{Z} e^{-\beta E_r}, \tag{9}$$

where $\beta = k_B T, k_B$ is the Boltzmann constant, T is the system's temperature and $e^{-\beta E_r}$ is the Boltzmann weight. This probability distribution is called the Boltzman-distribution. The partition function Z normalizes the Boltzmann distribution with:

$$Z = \sum_r e^{-\beta E_r} \tag{10}$$

There are many methods for defining the partition function [**18**]. We are considering the recursive relations method. In this method the lattice is cut into branches and the total partition function is expressed in terms of the reduced partition functions of all branches. This procedure allows to derive a one or multi -dimensional mappings for the branches of the partition function, thus providing a recursive relation in particular for such a property as a magnetization.

The partition function Z of our model can be expressed by the following formula:

$$Z_{IH} = \sum e^{-\beta H_{IH}} = \sum_{\mu_0} e^{-\frac{\Delta(\mu_0^z)^2 - g\mu_B h \mu_0^z}{k_B T}} g_n\,(\mu_0^z)^2, \tag{11}$$

where μ_0 denotes the central spin and $g_n(\mu_0)$ is a contribution to the partition function of one lattice branch, starting from the central site with fixed spin value μ_0 (see Figure 2.). $g_n(\mu_0)$ is connected with $g_{n-1}(\mu_1)$ by the following equation:

$$g_n\,(\mu_0) = \sum \exp((J(S_1S_2 + S_1S_3 + S_2S_3) + J_1(S_1 + S_2 + S_3)(\mu_0 + \mu_1) + \Delta\left(S_1^2 + S_2^2 + S_3^2 + \mu_1^2\right) - g\mu_B h(S_1 + S_2 + S_3 + \mu_1))/k_B T) g_{n-1}\,(\mu_1) \tag{12}$$

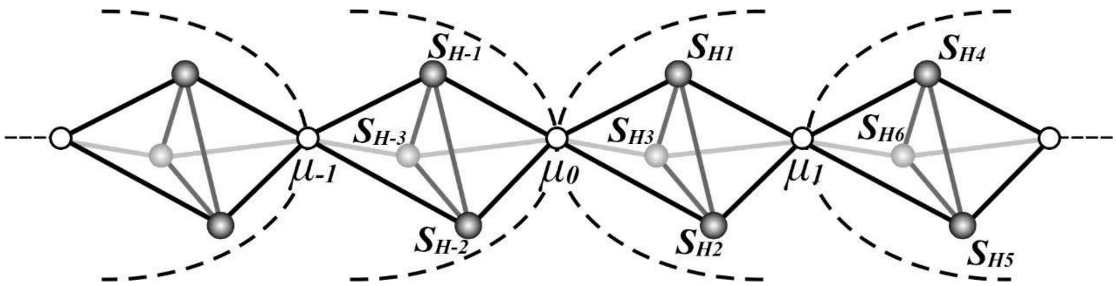

Figure 2.
The schematic of the partitioned double tetrahedral chain

Let us introduce new notations:

$$x_n = \frac{g_n\,(1)}{g_n\,(0)}, y_n = \frac{g_n\,(-1)}{g_n\,(0)}, \tag{13}$$

By inserting $g_n\,(\mu_0)$ into equation (13) we get a set of recursion functions:

$$x_{n+1} = f_1\,(x_n\ , y_n)\,, \quad y_{n+1} = f_2\,(x_n, y_n)\,, \tag{14}$$

where $f_1\,(x, y\ )$ and $f_2\,(x, y\ )$ have the following form :

$$f_1\,(x,\ y) = \frac{a_0 + a_1 x + a_2 y}{c_0 + c_1 x + c_2 y}, f_2\,(x,\ y) = \frac{b_0 + b_1 x + b_2 y}{c_0 + c_1 x + c_2 y} \tag{15}$$

Journal of Physics: Conference Series **2912** (2024) 012038 doi:10.1088/1742-6596/2912/1/012038

4 Lyapunov Exponents

Lyapunov characteristic exponents (briefly LCES, also called Lyapunov characteristic numbers or simply characteristic exponents) play an important role when the stochastic properties of dynamical systems are studied both from a theoretical and a numerical point of view. It is interesting to apply Lyapunov exponents connecting with magnetization plateau and magnetic susceptibility with antiferromagnetic couplings at low temperatures ($T \to 0$). Lyapunov exponents, characterize the degree of the exponential divergence of two neighboring points induced by the mapping presented by equation (14). They provide a measure of the degree of "instability" of the system: a positive maximum Lyapunov exponent corresponds to chaotic, unstable states, while a negative maximum Lyapunov exponent signals stable states. If we have a dimensional map then a spectrum of exponents is present [**8**],[**16**], [**18-20**]. The Lyapunov exponent is calculated by the following equation:

$$\lambda_{\mathbf{1,2}} = \lim_{N\longrightarrow\infty} \frac{1}{N}\, ln\left(eigenvalues\left\{\Lambda\left(x_1,\ y_1\right),\ \Lambda\left(x_2,\ y_2\right)\cdots\Lambda\left(x_N,\ y_N\right)\right\}\right)$$

where $\Lambda\left(x_i,\ y_i\right)$ is a Jacobian matrix evaluated at the $(x_i,\ y_i)$ point.

$$\Lambda\left(x_i,\ y_i\right) = \left(\begin{array}{cc} \frac{\partial f_1}{\partial x} & \frac{\partial f_1}{\partial y} \\ \frac{\partial f_2}{\partial x} & \frac{\partial f_2}{\partial y} \end{array}\right)_{x_i,\ y_i}$$

We used a standard (Gram-Schmidt) numerical procedure to compute both Lyapunov exponents for our 2-dimensional recursion relations. We consider a point as super-stable if it's maximum Lyapunov exponent tends to minus infinity when the temperature goes to zero (see figures below).

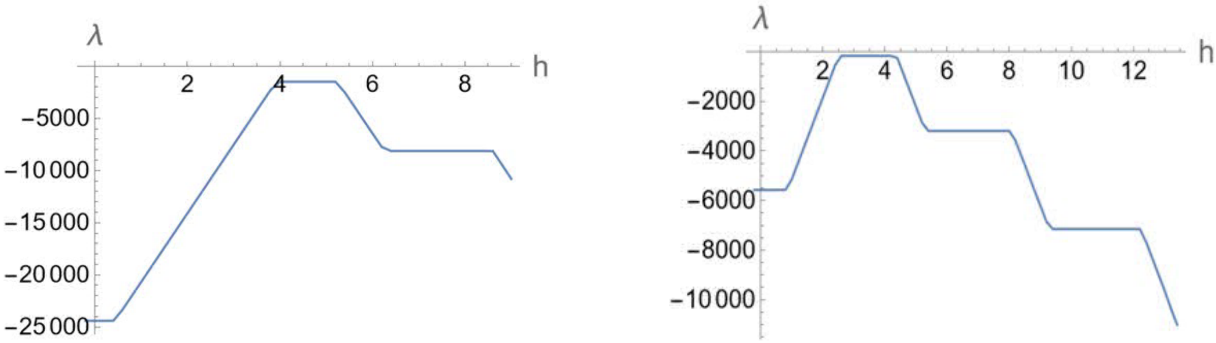

Figure 3. Super-chain for Δ=5; J=3; J_1=0.5; T=0.0005 (left) and Δ=3; J=3; J_1=1; T=0.001 (right)

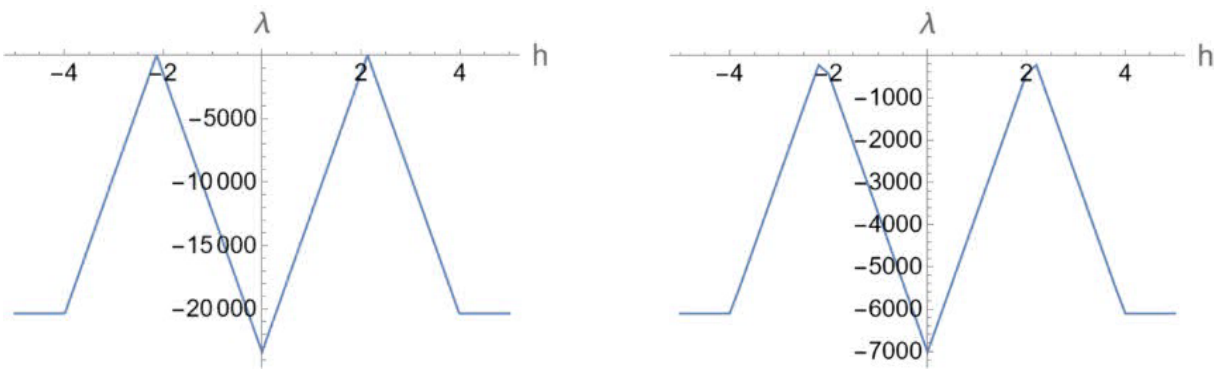

Figure 4. Super-stable points for Δ=3; J=3; J_1=-0.5; T=0.0003 (left) and Δ=3; J=3; J_1=-0.5; T=0.001 (right)

Journal of Physics: Conference Series **2912** (2024) 012038 doi:10.1088/1742-6596/2912/1/012038

5 Conclusion

Using recursive relations method for definition of the partition function and applying Lyapunov exponents, we find super-stable points and super-stable cycles for double-tetrahedral chains, when the temperature tends to zero. Our further studies will aim to show symmetry between super-stable chains and magnetization plateaus.

6 Aknowledgments

G. A., N. A., H.P., L.A. acknowledge the receipt of a grant in frame of the research project 21AG-1C006: "Quantum Magnetic Properties, Correlations, Thermal Entanglement of Metal Containing Compounds" and project 23SC-CNR-1C006: "Thermodynamics and many-body correlations of quantum magnets".
.

References

[1] Zheng Yi-Dan, Mao Zhu, Zhou Bin 2017 *Chinese Physics B* **26** 070302

[2] Ananikian N, Strecka J and Hovhannisyan V 2014 *Solid State Commun.* **194** 48

[3] Canov L, Strečka J and Jăsčur M 2006 *Solid State Commun.* **18** 4967

[4] Abgaryan V, Ananikian N, Ananikyan L and Hovhannisyan V 2015 *Solid State Commun.* **224** 1

[5] Amatuni G, Burdik Č, Poghosyan H, Ananikyan L and Ananikian N 2023 *Journal of Physics: Conference Series* **2667** 012062

[6] Krupnitska A 2020 *Physical Review B* **102** 064403

[7] Silva da Conceição C and Maia R 2017 *Physical Review E* **96**, 032121

[8] Lee M 2014 *Commun.Theor. Phys.* **62** 485

[9] Lee M 2009 *J. Math. Phys.* **50** 122702 122702

[10] Ananikian N, Ananikyan L, Artuso R and Lazaryan H 2010 *Physics Letters A* **374** 4084

[11] Strogatz S 2014 *Nonlinear Dynamics and Chaos: With Applications to Physics, Biology, Chemistry, and Engineering, Studies in Nonlinearity (Colorado:Westview Press)*

[12] Smale S 2013 *The Mathematics of Time: Essays on Dynamical Systems, Economic Processes, and Related Topics (New York:Springer-Verlag)*

[13] Thirring W 1992 *A Course in Mathematical Physics 1 and 2 (New York:Springer)*

[14] Ananikian N, Artuso R and Chakhmakhchyan L 2014 *Commun Nonlinear Sci Numer Simuln* **19** 3671

[15] Ananikian N, Ananikyan L and Chakhmakhchyan L 2011 *JETP Letters* **94** 39

[16] Ananikian N and Hovhannisyan V 2013 *Physica A* **392** 2375

[17] Ananikian N and Dallakian S 1997 *Physica D:Nonlinear Phenomena* **107** 75

[18] Hovhannisyan V, Strečka J and Ananikian N 2016 *J. Phys.: Condens. Matter* **28** 085401

[19] Ananikian N, Artuso R and Poghosyan H 2018 *Physica A* **374** 892

[20] Ananikian N, Burdik Č, Ananikyan L and Poghosyan H 2017 *J. Phys.: Conf. Ser* **804** 012022