Order-by-disorder in a SU(4) Heisenberg model on a FCC lattice

and

generalized Kac lemma for recurrence time in iterated open quantum systems

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Theses of the dissertation

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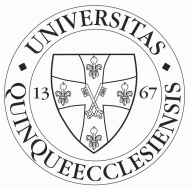

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(2016)

1. Antecedents and motivations of our work

1.1. Average recovery time in physical systems

The need for scientific theories was demanded by the observation of the surrounding macroscopic events happening from time to time. Such periodic events were for example the alternation of days and nights, or the passage and recurrence of the seasons. The observed regularities suggest the existence of underlying natural law or laws. Taking Earth's circulation and rotation into account is necessary for an explanation of the presented examples. These arguments were already known in ancient cultures as well, who further noticed that with the passing of a year the Earth does not return to its exact prior position but to one very close to it. Their notes however concluded that the Earth after all does return to its initial place and this time elapsed is called "Great Year" or "Platonic Year". The then most accurate calculations carried out by the Babylonians, who identified one year as 360 days(hence the partition of the total circle into 360 degrees) while the Great Year is 36,000 years[1, 2, 3].

Newton in his work[4] (published in 1687) seemingly gave a complete explanation of the movements of all the planets found in the solar system but the efforts to find a concrete solution for the systems consisting of two bodies remained unsuccessful. The simplest of the unresolved problems was the three bodies problem for which by the end of the 19th century there were some approximate solutions bound to initial conditions however the existence of an exact solution remained an open question. Upon the invitation of II. Oscar Swedish king in 1887 Poincaré started to work on this minimal problem however his efforts were unsuccessful. He concluded that the problem can not be solved in a close form. His win of the prize was further supported by the other two positive results he found, 1) He showed that a small change in the initial conditions, in an unpredicted manner, results in a fairly large change in

the solution to which sensitivity we have to pay attention to in our calculations. (This remark lead to the birth of the chaos-theory.) 2) Beyond the specific problem he proved that when in a process the certainty equivalent of a state is a constant, a system returns to almost every previous state after a certain time (Poincare time)[7, 8, 9].

On the magnitude and average frequency of returns of the returning time introduced by him Poincaré made no estimates. For this we had to wait until 1947, when Kac also proved that if a state is recurrent then it is indeed infinitely recurring, whilst using the lemma named after him to determine the average return time of a state. According to Kac lemma the average return time of a state is equal to the reciprocal of its equilibrium distribution[10]. I have further discussed the strength of the lemma in the thesis hence now I will only demonstrate one of its unusual applications. Compare the frequency of occurrence of 7 and 8 (in the decimal numeral system) in the first digit of the 2^n ($n \in \mathbb{N}$) series, as well as the average number of steps until the first digit becomes 7 and then 8 again. All members of the series can be written in the form of $2^n = B \cdot 10^k$ where $1 \leq B < 10$ and $k \in \mathbb{N}$. Thus if $7 \leq B < 8$ the given member of the series starts with 7, when $8 \leq B < 9$ the first digit of the first element is 8. Taking the logarithm of the basis of 10 of the previous form we obtain the following: $n\log(2) = k + \log(B)$. Hence to get the first digit of every element take n times $\log(2)$ ignoring its integer parts, and see which two integers' logarithms it falls between (if the result falls in the interval of $[\log(7), \log(8))$ the first element of the series starts with 7. Considering that $0 \leq \log(B) \leq 1$, multiplying both sides with 2π the original problem can be replicated to a rotation on a unit circle, where the unit rotation is defined by the angle that has the size $2\pi\log(2)$. Thus the equilibrium distribution of the first digit of the elements is determined by the length of the arc, normalized with 2π, on the unit circle, assigned to them, from which the probability that the first digit of $2n$ be 7 is: $P_7 = \log(8) - \log(7) \simeq 0.058$, similarly $P_8 \simeq \log(9) - \log(8) = 0.051$.

From the Kac lemma we know that in average every member with the first digit of 7 will be followed by another in $N_7 \simeq 1/0.058 \simeq 17.24$ steps, while in the case of 8 this number is $N_8 \simeq 1/0.051 \simeq 19.6$. Note that the prior result (apart from some specific power bases) is universal.

Moving away from the description of macroscopic systems the definition explaining the dynamics of the system has to be modified. Hence while in some classical systems the evolution of time can be described by the iterative use of given transfer matrices, in a closed system of the quantum world these dynamics are described by a unitary operator's iterated use. Furthermore whilst in the classical systems the definition of the average first return time did not pose any problems, in the quantum world this step can not be performed in a well defined way, since we have to ensure the avoidance of multiple returns, which requires some sort of interference. One way to interfere is to monitor continuously, so we modify the dynamics in the following way: We measure the system after every step, and if it returned to the ground state, we stop the process. The time necessary to stop the process is identified by the return time of the process, and the return times given by this method will unequivocally lead to the first average return time by making a statistical averaging over them Grünbaum et al. in 2013 found that the average return time of an arbitrarily chosen state of an arbitrary closed physical system is an integer or infinite[11].

1.2. Ground state of the SU(N) Heisenberg model

On an adequately low temperature certain degrees of freedom of condensate materials freeze out, thus they present distinct structure and collective properties. For instance until we examine these on a temperature lower than the energy of the U interaction between its particles and according to the $K_B T$ energy, they can be regarded as crystallized materials. The electricity flowing in these crystals, with spin- or orbital angular momentum a uniform magnetic behavior can develop, this

certain solid-states (even without an external magnetic field) can have an induced magnetic field. These materials are referred to as ferrite magnets and their corresponding transformation temperature is called Curie-temperature[12]. The following graphic image can be associated with the ferromagnets: to every grid of the crystal an elementary magnet is assigned, that point in the same direction on every grid, while in the ferromagnets the elementary magnets point in different directions and the macroscopic magnetism of the crystal is given by the changing strength of the elementary magnets[13]. The other large group of magnetic materials is formed by diamagnets, paramagnets and antiferromagnets, since in these a spontaneous induced magnetic field does not occur. Diamagnetism create an induced magnetic field in a direction opposite to an externally applied magnetic field, whilst in paramagnets the induced field is created in the same direction as the externally applied field. In antiferromagnets the neighboring grids exhibit a magnetic ordering in opposing directions, however unlike in the ferromagnets here the elementary magnets have the same strength[14, 15, 16].

The whole spin of elementary magnets formed on a grid point of a solid, can originate from the kernel or the magnetic or orbital angular momentum of the electrons, as well as due to the surrounding momentums' shading effect it may also shorten. To model the interaction of these momenta the isotropic Heisenberg-model is appropriate, which takes into account the Pauli-principle and the direct and kinetic exchange mechanisms. The Heisenberg-model describes the interaction of the spins of the solid-states as a sum of coupled interactions, between which the J connection is regarded as grid independent. Assuming these pair interactions are unable to induce the atom which carries the spin of the grid hence we focus on the spin rotating role of each interacting parts that are sufficient to describe the coupled interactions. According to the model's J parameter's sign, in the crystal a ferromagnetic ($J < 0$), or an antiferromagnetic ($J > 0$) ordering is preferred.

Despite its apparent simplicity, the Heisenberg-model describes the surrounding physical systems well, in addition apart from some special cases an exact solution does not exist. When examining the ground-state of the model we came across a variety of exotic phases, which is mainly influenced by the lattice that belongs to the model and the size of the spin of the grids. First, in 1944 L. Onsager proved with his exact calculations that the initial state of an SU(2) Heisenberg-model placed on a square lattice can also be an ordered phase[17, 18]. Following this, the examination of the symmetry properties of the ground state of the SU(N) symmetric Heisenberg-model began[19, 20, 21, 22, 23, 24, 25]. The individual results have shown that in infinitely large systems the ground state can be arbitrarily close to the Néel-ordering, furthermore the deviation from these orderings increases with the decreasing of the grid size. Hence by the examination of a finite but sufficiently large system the initial state (in certain parameter ranges) can be approximated by a classical Néel-ordering. However when determining the ground state we have to take the Mermin-Wagner theorem into account, which states that at a finite temperature there has to be a minimum of two dimensions for an ordering to be formed in the ground state [26, 27, 28].

2. Summary of results

2.1. The average first return time of open quantum systems

We were inspired to work on open systems by an article published in 2013 where Grunbaum et al gives a quite technical, topological argument in this article, that in iterated unitary dynamics, the system returns to its initial state in integer or infinite steps (in average) . We interconnected this problem with a theorem known in classical dynamics, which states that in doubly stochastic iterated dynamics, the average

return time is equal to the size of the irreducible graph associated with the initial state. We further generalized our theorem which was named as the quantum Kac lemma.

With the investigation of open systems, we had the chance to connect purely quantum and purely classical systems, with a continuous d decoherence parameter, where $d = 0$ corresponds to a purely quantum system, while $d = 1$ results in a purely classical system. The time development of a quantum system can generally be given by a quantum channel. The Kraus representation of this channel presumes a constant environment through time-development. With the introduction of this dynamics, we were able to link the two doubly stochastic limits, (i.e., the doubly stochastic classical dynamics and the unitary dynamics), and to show that if the dynamics is unital (in both limits), than the average return time stays quantized and is equal to the dimension of the Hilbert space explored by the system We investigated the applicability and the surprising behaviour of the theorem we got[III]. We displayed the robustness of the problem by exploring the 'relevant Hilbert space' through several examples.

As I dug deeper in this field, I have realised that if a system's initial state is an eigenstate of the equilibrium density operator, then the average returning time can be calculated from the system's equilibrium distribution[I]. In the previous special cases this condition is automatically satisfied, since in those cases the equilibrium distribution is the multiple of the unit operator. According to the found theorem the reciprocal of the number we get by the normalization of the state gives exactly the average returning time (which is in accordance with the results we got using for unital dynamics). Our theorem given by these more general dynamics, at the classical extremes is the same as the classical Kac theorem. Finally, we showed through an example, that the found quantum Kac lemma is applicable to find the average hitting time between arbitrary states in every iterated dynamics driven system,

where we use a classical tool to determine if the walker hits the target state or not[I].

2.2. SU(4) symmetric anti-ferromagnetic Heisenberg model on an fcc lattice

I have started to investigate the spin systems in my MSc thesis, and now I continue do so as a PhD student. In the course of investigating these systems, I have always aimed to understand the SU(N) spin operators' different representations and applications. We examined two physically different model: one being the SU(6) symmetric anti-ferromagnetic Heisenberg model on a hexagonal lattice**??**, and the other being the SU(4) symmetric antiferromagnetic Heisenberg-model on an fcc lattice[II]. We used different representations in the two mentioned models, because we expected different outcomes. We expected an SU(6) symmetric spin-liquid ground state in the first model, while an ordered phase in the second one. As the results of our research on the first model has already been presented in my MSc thesis, I concentrated on the second one in my doctoral thesis.

We chose the boson representations of the spin operators in the course of investigating the ordered phase, since in the ground state, they Bose-condensate, so they violate the SU(4) rotational symmetry. This representation of spins results in a four operator interaction term which in general cannot be treated in an exact way, so we used the 'spin wave approximation' to handle this term. In the first step of this approximation we determined all the possible classical configurations of the (degenerate) ground state. We found in the course of the calculations, that this ordering is not unique. For simplicity, we chose a one parameter ensemble (helical states) from these possible states, and tried to find the model's ground state on this subspace. To carry out this approximation, we need the boson operator's Holstein-Primakoff representation, where we used the semiclassical series expansion. With the help of the

series expansion, the degeneracy of the classical states splits up, and only one state remained as the ground state of the system. This type of the selection is called as the “order-by-disorder” mechanism. We made a stability analysis of the obtained ground state by calculating the spin reduction, as a self-consistency condition being satisfied, i.e., in the semiclassical approximation we put forward as a hypothesis, that the magnetization on each lattice site has a well defined, classical direction which can only change a little due to perturbations. These quantitative checks showed, that at a finite temperature, the obtained phase becomes unstable, which can be explained graphically as the Mermin-Wagner theorem prevents the obtained phase behaving as a quasi 2 dimensional system. The higher orders of the approximation were taken into account as an effective ferromagnetic Heisenberg interaction between the next nearest neighbors, and so we calibrated the value of the coupling accordingly. In the extended model we found that the obtained ground state stabilized even on a finite temperature.

Finally, we determined the spin-spin correlation function for the helical states (characterized by the ϑ parameter) by this quantity the spin configurations of the state can be identified, with the help of the scattering experiments.

3. Publications

3.1. Publications included in the current thesis

[I] Sinkovicz P., Kiss T., Asbóth J. K. – Generalized Kac's Lemma for Recurrence Time in Iterated Open Quantum Systems, **Phys. Rev. A**, 93. 050101(R) (2016) /impaktfaktor: 2.81/

[II] Sinkovicz P., Szirmai G., Penc K. – Order by disorder in a four flavor Mott-insulator on the fcc lattice, **Phys. Rev. B**, 93. 075137 (2016) /impaktfaktor: 3.74/

[III] Sinkovicz P., Kurucz Z., Kiss T., Asbóth J. K. – Quantized recurrence time in iterated open quantum dynamics, **Phys. Rev. A** 91. 042108 (2015) /impaktfaktor: 2.81/

3.2. Publications not included in the current thesis

[IV] Sinkovicz P., Zamora A., Szirmai E., Lewenstein M., Szirmai G. – Spin liquid phases of alkaline-earth-metal atoms at finite temperature, **Phys. Rev. A** 88. 043619 (2013) /impaktfaktor: 2.99/

[V] Szoboszlai Z., Nagy Gy., Kertész Zs., Angyal A., Furu E., Török Zs., Ratter K., Sinkovicz P., Kiss A.Z. – Characterization of atmospheric aerosols in different indoor environments, **ATOMKI Annual Report**, ISSN 0231-3596 (no.26) 43, 41., 43102323 (2011)

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