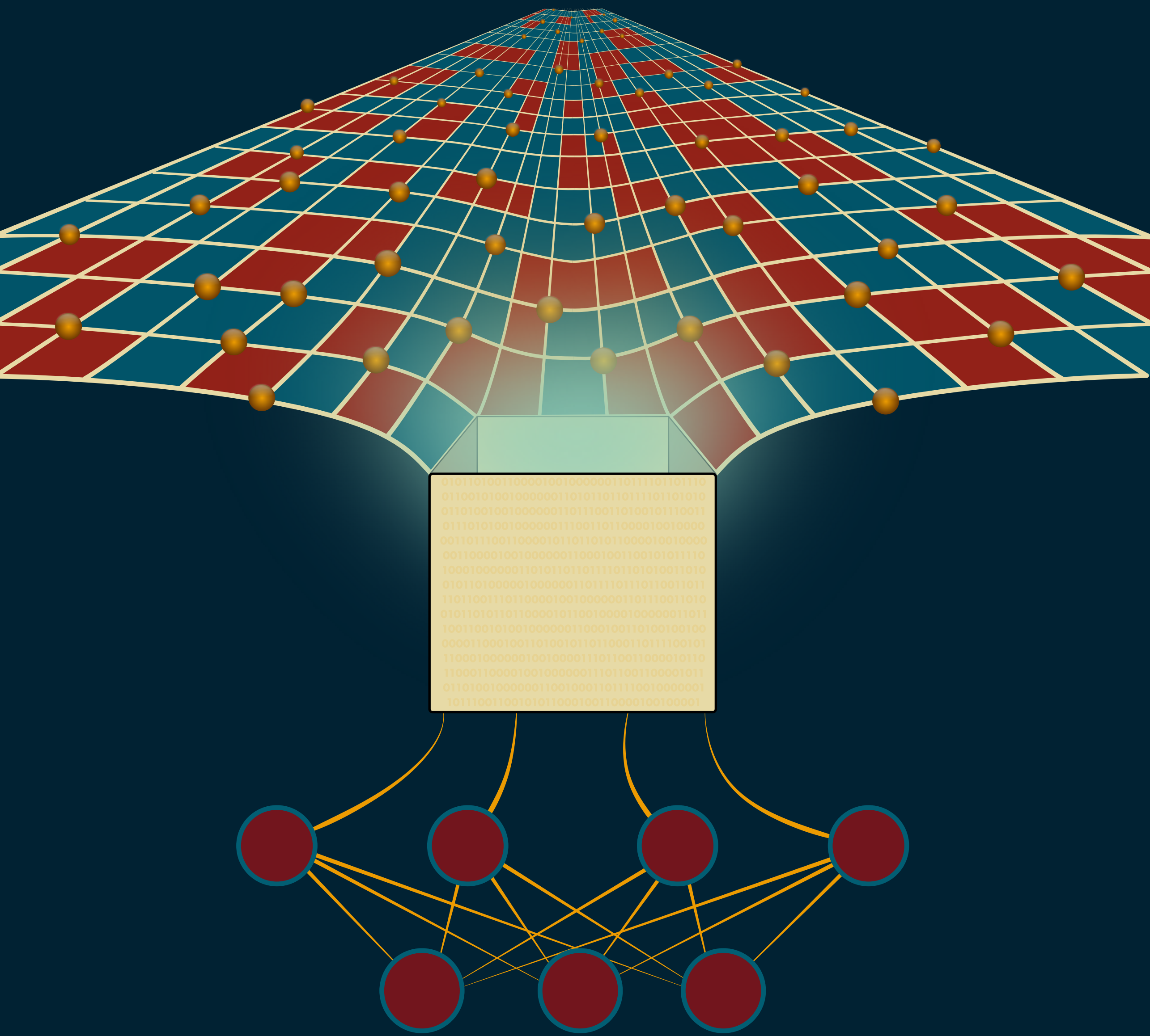
Numerical Exploration of Statistical Physics



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Numerical Exploration of Statistical Physics

Proefschrift

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The cover was created by me, representing the synergy of the whole thesis in a single image.

Contents

Samenvatting

Vooruitgang op het gebied van computerhardware wordt doorgaans opgevolgd door toepassingen die proberen de nieuwe hardware maximaal te benutten. Deze vooruitgangen vinden ook hun weg naar de wetenschap, waar ze ons helpen om de bestaande grenzen van wat mogelijk is te verleggen.

Aan het begin van dit proefschrift, in hoofdstuk 2, contrasteren we de huidige consensus over thermalisatie in gesloten kwantumsystemen, de “eigentoestand thermalisatie hypothese” (ETH), tegenover een recent ontdekte “operator thermalisatie hypothese” (OTH), doormiddel van het bestuderen van thermalisatiedynamiek in gesloten unitaire kwantumsystemen. We hebben aangetoond hoe de twee hypotheses verschillend zijn, en toch in sommige opzichten vergelijkbaar. No-go-voorwaarden die worden opgelegd door de OTH zijn een kenmerk van de integreerbaarheid van de theorie, en slechts een kleine beweging van deze voorwaarden vandaan zorgt ervoor dat de matrixelementen hun ETH-vorm benaderen. Voor het oplossen van deze grote “eigen-problems” was rekenkracht nodig van het lokale computerraster van de Universiteit Leiden.

Een van de meest alomtegenwoordige numerieke methoden in de wetenschap is de Monte Carlo-simulatie, oorspronkelijk ontwikkeld door Stanisław Ulam toen hij werkte aan kernwapens in het Los Alamos National Laboratory. De hoofdgedachte van Monte Carlo simulatie is het willekeurig nemen van steekproeven van de waarden van een integrand om bij benadering de waarde van een integraal te berekenen. Hiermee heeft Monte Carlo-simulatie heeft een revolutie teweeggebracht in de wetenschap en het hedendaagse computing. In hoofdstuk 3 bestuderen we de zogenaamde “rooster-ijktheorie”. Voortbouwend op de fundamenten die Wegner heeft gelegd bij zijn realisatie van de pure Z_2-ijktheorie, en een uitbreiding van het werk van Fradkin en Shenker, construeren we Z_2-ijktheorie gekoppeld aan de verschillende materievelden. Ondanks het feit dat ze niet interageren, leiden deze materievelden tot interessante verschijnselen wanneer ze worden doorgemeten met hetzelfde ijkveld. Er is namelijk een nieuwe “registry” -orde in de Higgs-fase ontstaan, wat betekent dat lokaal verschillende kopieën van materievelden hun vectoren parallel en anti-parallel uitlijnen, zelfs in de aanwezigheid van continue $O(2)$-symmetrie van materie velden.

Door Monte Carlo-simulaties uit te voeren voor grotere 3D-roosters hebben we een aantal interessante kenmerken ontdekt van faseovergangen die voorheen overschaduwd werden door de effecten van eindige grootte.

De afgelopen jaren zijn we getuige geweest van een overweldigende ontwikkeling van machine learning-technieken, geïnspireerd door de nieuwe generaties grafische kaarten. De industrie leidde voornamelijk het onderzoek naar nieuwe toepassingen; toch hebben deze nieuwe en enerverende toepassingen hun weg gevonden naar de wetenschap, vooral de natuurkunde. Een ~~Samenvatting~~ methode, “gedoopte” neurale kwantumtoestanden (NQS), overweegt het gebruik van een neuraal netwerk om toestanden van zeer verstrengelde kwantum toestanden te representeren. Een bijzondere architectuur van neurale netwerken, genaamd “Restricted Boltzmann-machines” (RBM), is zeer geschikt voor de taak, gedeeltelijk omdat het niet-lokale correlatie dankzij het ontwerp omvat. In hoofdstuk 4 onderzoeken we verstrengelingsentropie en de schaling ervan voor dezelfde ijktheorieën als in hoofdstuk 3, nu uitgedrukt als een 2D-kwantumtheorie in één dimensie lager. We stellen vast dat de verwachte lineaire relatie tussen het totale aantal materievelden en verstrengelingsentropie niet aanwezig is.

De manier waarop de natuurkunde de toepassingen van machine learning heeft omarmd, kan ook andersom worden gebruikt, om enkele van de successen te rechtvaardigen en deze verder te verbeteren. In navolging van deze mantra passen we in hoofdstuk 5 de inzichten uit de statistische fysica toe om de computationele mechanica van diepe neurale netwerken te bestuderen. We onderzoeken de wijze waarop de initiële parameterverdeling voor de gewichten en biases kan leiden naar twee verschillende faseregimes van het netwerk, en hoe het kiezen van het optimale punt binnen dit fasediagram de uiteindelijke nauwkeurigheid van het netwerk bepaalt, onder de voorwaarde van een gelijke trainingstijd. We stellen vast dat het initialiseren van gewichten en biases volgens de lijn van faseovergang een noodzakelijke maar geen voldoende voorwaarde is voor optimale trainbaarheid.

Summary

Advancements in computing hardware are usually followed by emerging applications trying to utilize the new hardware to the maximum. These advances also find their way into science, where they help us push the boundaries of what has been possible so far.

At the beginning of the thesis, in Chapter 2, we contrast the current consensus answer about thermalization in closed quantum systems, the eigenstate thermalization hypothesis (ETH), with a recently discovered operator thermalization hypothesis (OTH) by studying thermalization dynamics in closed unitary quantum systems. We showed how the two are different and yet similar in some regards. No-go conditions imposed by the operator thermalization hypothesis are a feature of the integrability of the theory, and just a slight move away from it would make matrix elements approach their ETH form. Solving these big eigen problems required the firepower of the local computing grid at Leiden University.

One of the most ubiquitous numerical methods in science is Monte Carlo simulation, initially developed by Stanisław Ulam while working on nuclear weapons at Los Alamos National Laboratory. The main idea of Monte Carlo is to randomly sample the values of an integrand to compute the approximate value of an integral, revolutionized science and modern-day computing. In Chapter 3, we turn to the lattice gauge theory. Building on the foundations set by Wegner in his realization of the pure Z_2 gauge theory and expanding the work of Fradkin and Shenker, we construct Z_2 gauge theory coupled to the several matter fields. Even though they are non-interacting, these matter fields lead to exciting phenomena when gauged through the same gauge field. Namely, a new "registry" order in the Higgs phase has emerged, meaning that locally different copies of matter fields align their vectors in a parallel and anti-parallel fashion, even in the case of continuous $O(2)$ symmetry of matter fields. Running Monte Carlo simulations for bigger 3D lattice sizes, we have discovered some exciting characteristics of phase transitions previously obscured by the finite-size effects.

In recent years we have witnessed an overwhelming development of machine-learning techniques inspired by the new generations of graphic cards. The industry predominantly led the research of new applications; nevertheless, these new and exciting applications have found their way into science, especially physics. One

method, dabbed neural quantum states (NQS), considers using a neural network to represent a quantum state of highly entangled systems. A particular architecture of neural networks called Restricted Boltzmann machines (RBM) is very well situated for the task, partially because it includes non-local correlation by design. In Chapter 4, we explore the entanglement entropy and its scaling of the same gauge theories from Chapter 3, now expressed as a 2D quantum theory in one lower dimension. We find that the expected linear relation between the total number of matter fields and entanglement entropy is not present.

In the same way, that physics has embraced applications of machine learning, it also can be used the other way around, to justify some of its successes and further improve upon them. Following this mantra in Chapter 5 we apply the insights from statistical physics to study the computational mechanics of deep neural networks. Precisely how the initial parameter distribution for the weights and biases can lead to two different phase regimes of the network and how choosing the optimal point in this phase diagram can make the final accuracy of the network change given equal training time. We find that initializing weights and biases along the line of phase transition is necessary but not sufficient condition for optimal trainability.

List of Publications

1. “ New approaches for boosting to uniformity”,

   A. Rogozhnikov, **A. Bukva**, V. Gligorov, A. Ustyuzhanin and M. Williams
   JINST, 11 (2015) T03002.

2. “Operator thermalization vs eigenstate thermalization”,

   A. Bukva, Philippe Sabella-Garnier, Koenraad Schalm,
   e-Print: 1911.06292.

3. “Criticality versus uniformity in deep neural networks”,

   Aleksandar Bukva, Jurriaan de Gier, Kevin T. Grosvenor, Ro Jefferson, Koenraad Schalm, Eliot Schwander
   e-Print: 2304.04784, submitted to *JMLR*.

4. “Replicating Higgs fields in Ising gauge theory: the registry order”,

   Aleksandar Bukva, Koenraad Schalm, Jan Zaanen
   e-Print: 2305.02400, submitted to *Phys.Rev.E*.

Curriculum Vitae

I took my first breath on May 20th, 1994, in Kikinda, a small city in the north of Serbia. After finishing elementary school in Kikinda, I moved to Novi Sad to attend one of Serbia's best and oldest high schools, gymnasium Jovan Jovanovic Zmaj.

High school was the place where I discovered that I wanted to study physics later in life. Besides the regular high school curriculum, I attended the physics seminar at Petnica science center. I was quickly introduced to the world of computer simulations and developed a particle-in-cell (PIC) code for simulating a plasma wave accelerator. After finishing high school, I moved to Belgrade, where I obtained my bachelor's degree. In the first year, my publication "New Approaches for Boosting to Uniformity" was awarded the best technical paper at Belgrade University. During my bachelor's, I continued my interest in computational physics. I did a summer internship at Helmholtz-Zentrum Dresden Rossendorf in a group of Dr. Michael Bussmann, where I worked on an improved version of an integration algorithm for their PIC code.

I continued my master's degree in Belgrade. Still, I did most of my thesis work at the Institute of Physics under the supervision of Milica Milovanović. The title of my master's thesis is: "Lattice-like structures in Lowest Landau Level" where we were trying to construct an effective Hamiltonian for a bosonic system on a square lattice that will support fractional quantum Hall effect (FQHE) at $\nu = \frac{1}{2}$. I started my Ph.D. in November 2018, in the Quantum Matter Theory Group at the Lorentz Institute of Leiden University, under the supervision of Prof. Dr. J. Zaanen and Prof. Dr. K.E. Schalm. During my Ph.D., I taught a couple of courses as a teaching assistant, "Classical Electrodynamics" and "Theory of General Relativity". Alongside the research, I have attended several schools during my Ph.D., DRSTP Schools in High Energy and Condensed Matter Physics, in Brazil and the Netherlands. I have also presented my work at several Physics@Veldhoven conferences.

As of January 1st, 2023, I have started working as a Quantitative Developer for an energy trading company Northpool B.V.

Acknowledgements

This thesis is a culmination of all the work done and events that happened since I moved to the Netherlands. First, I would like to thank Jan Zaanen and Koneraad Schalm for their guidance on this journey and all the knowledge they shared during that time.

Even though there is a single name on this thesis, people in my research group have helped me a lot through numerous discussions, code debugging, and brainstorming; thank you a lot, in no particular order, Vladimir Ohanesjan, Aravindh Swaminathan Shankar, Floris Balm, Nicolas Chagnet, Tereza Vakhtel, Philippe Sabella-Garnier, Kevin Grosvenor, Vincenzo Scopelliti and Aurelio Romero-Bermudez. Also, thank you for making these years in Leiden very enjoyable.

I would also like to express my gratitude to my friends, with whom I have also discussed some of the problems that I've encountered while working on this thesis, thank you Marko Kuzmanović, Daniel Szilagyi, Ognjen Stanisavljević and Dušan Drobnjak.

I also want to thank the support staff, the secretariat, and the IT of the Lorentz Institute and LION for their help. I would also like to thank the surfSARA, Alice cluster, and Xmaris personnel for the access to their compute resources, without which none of the results in this thesis would be possible.

And finally, from the bottom of my heart, I would like to thank my mom, dad, and brother for all the support they gave me. Without your it, none of this would be possible. Puno vam hvala!

Stellingen

Behorende bij het proefschrift

Numerical Exploration of Statistical Physics

1. Integrable theories can have operators that thermalize.

   [*Chapter 2*]

2. Multiple matter fields gauged with the same Z_2 field exhibit "registry" order parameter in the Higgs phase.

   [*Chapter 3*]

3. Entanglement entropy of the lattice gauge theories with matter fields at criticality does not grow with the number of additional matter fields.

   [*Chapter 4*]

4. Initialization along the edge of chaos is a necessary but not sufficient condition for optimal trainability.

   [*Chapter 5*]

5. Generative models can be used to improve calculation of entanglement entropy in lattice gauge field models.

   M. Medvidovic, J. Carrasquilla, L. E. Hayward, B. Kulchytskyy, *Generative models for sampling of lattice field theories* arXiv:cond-mat/2012.01442

6. The recent development of machine learning techniques can significantly improve our current optimization algorithms. But caution must be applied and methods understood rather than mindlessly used.

7. Advancements in computational physics would be vastly accelerated by making codes of research papers publicly available.

8. The accuracy of the ground-state energy is not sufficient evidence of the proper representation of a ground state in gapless systems.

9. Considering machine learning beyond being merely a profoundly intricate minimization challenge is fruitless.

Aleksandar Bukva
Leiden, 10th October 2023