PhD project description

"Machine learning localized and many-body localized quantum Hamiltonians" – Rudolf A Roemer

Disordered quantum systems continue to play a key role in theoretical developments of modern condensed matter physics. Originally, this is due to Anderson's realization in 1958 that the quantum wave nature of condensed matter can lead to interference effects that suppress the classically expected charge transport mechanisms – the birth of Anderson localization[1]. Already in Anderson's paper, it was discussed how the situation might be influenced by many-body effects. In the last decade, following the increase in computational power to allow the construction of meaningfully large Hilbert spaces even for interacting systems, this interplay of disorder and many-body physics has received much attention[2]. It was shown, numerically, that a novel transition seems to exist which separates thermalizing/ergodic states from non-thermalizing/localized states[3]. However, most results thus far are still based on standard BLAS/LaPack exact diagonalization techniques for very small real-space sizes of about 20 physics sites. On the other hand, when analytical results are available[4], these are for very strongly disordered systems where the presence of a localized phase in the presence of interactions are not surprising.

What really is needed is a novel approach at solving the underlying Schrödinger equations. Sparse-matrix methods seem to be a good starting point, but at present, they are simply used as brute-force methods without much thought given to their internal workings. Recently, machine learning and deep learning have emerged as numerical techniques that use strategies of artificial intelligence to predict outcomes of numerical experiments[5]. Methods such as U-Nets and Generalized adversarial networks (GANs) are able to produce seemingly innovative and creative images, audio and movies. Also, variational autoencoders (VAEs) can mimic fine details of physical images such as electron diffraction images[6]. One of the most intriguing benefits of these DL methods is that their predictions are often good approximations computed quickly and without the need for much computer memory (at least when their "training" has been completed). Such approximations to solutions are exactly what modern iterative sparse diagonalization routines need in their internal processes. For example, the iterative Jacobi-Davidson process, when coupled with an iterative LU decomposition, only needs a quick approximate solution of the inverse system of equations solution to the matrix resolvent[7]. It therefore seems possible to use DL techniques to speed up such sparse matrix codes to construct well-approximated eigenstates for very large system sizes.

In the PhD project, we want (i) to investigate the combination of DL and sparse diagonalization methods and then use these new methods to (ii) provide solutions to the eigenvalue problem of single-article Anderson models and (iii) study to the many-body problem in low-dimensional disordered spin-systems.

[1] P. W. Anderson, "Absence of Diffusion in Certain Random Lattices," *Phys. Rev.*, vol. 109, pp. 1492–1505, 1958.

[2] D. A. Abanin and Z. Papić, "Recent progress in many-body localization," *Ann. Phys.*, vol. 529, no. 7, p. 1700169, Jul. 2017.

[3] D. J. Luitz, N. Laflorencie, and F. Alet, "Many-body localization edge in the random-field Heisenberg chain," *Phys. Rev. B*, vol. 91, no. 8, p. 081103, Feb. 2015.

[4] J. Z. Imbrie, V. Ros, and A. Scardicchio, "Local integrals of motion in many-body localized systems," *Ann. Phys.*, vol. 529, no. 7, p. 1600278, Jul. 2017.

[5] P. Mehta *et al.*, "A high-bias, low-variance introduction to Machine Learning for physicists," *Phys. Rep.*, vol. 810, pp. 1–124, Mar. 2018.

[6] J. Partington, J. Thorn, R. Beanland, and R. A. Roemer, "Machine learning large-angle convergent-beam electron diffraction," *Preprint*, vol. 1, pp. 1–17.

[7] O. Schenk, M. Bollhöfer, and R. A. Römer, "On Large-Scale Diagonalization Techniques for the Anderson Model of Localization," *SIAM Rev.*, vol. 50, no. 1, pp. 91–112, Jan. 2008.

Student opportunity: the project should be good for the student (1000 characters max.) *

Machine learning (ML) and deep learning (DL) are statistical analysis techniques that use strategies of artificial intelligence to characterize complex data and extract deep information. In recent years, these techniques have begun to be used not only in traditional computer science test cases, but also in real world applications as well as, more recently, in areas of advanced physics. In condensed matter systems, such techniques give useful insight into Ising and spin ice models, low dimensional topological systems, strongly correlated systems, as well as material science applications. It is probably fair to say that ML and DL are quickly becoming standard tools to use in physics. Hence the project as outlined here will enable a PhD student to learn essential tools of the trade and to develop an essential toolkit on ML+DL that will serve them well in their future physics career. Alternatively, these methods are extremely saleable for any scientist wanting to establish himself or herself outside academia.

Strategic need: why is the studentship needed now and why is it important (1000 characters max.)?

I effectively "just" (due to Covid) returned from sabbatical year 2019-2020 at CY Advanced Studies at Cergy-Paris Universite, where I learned the basics of ML and DL methods and applications. In addition, I am co-supervising a student with the EUtopia partner Prof A Honecker from CY on image-type problems of ML. I am in discussions to start a ML/DL collaboration with Prof D Kotsinos from the Computer Science Department of CY (ETIS). In September, I co-organized with Prof Honecker a 2-day workshop on "Artificial intelligence, mathematics and physics" with much emphasis on the topics outlined in this PhD proposal. A new collaboration on using ML/DL methods to solve partial differential investigations has just been started with the industrial partner Inductiva Research Labs (https://inductiva.ai/), a Portugal-based ML start-up company founded by former Google Deep Mind researchers, amongst others. In addition, the first papers to emerge with me as co-author on using ML/DL in physics are now being written. Hence, the ground work has been and is being laid, now is the time to move to use that momentum to help a PhD student to profit from the work.

My current student, Ms Djenabou Bayo, is in her 3rd year now. In 2020, I was "1st on the reserve list", had candidates, but no funds as the reserve list was never funded. In 2019, "The panel noted that your strategic case would be very strong for next year (2020 entry)". I did not apply in 2018, as I had received a "fresh" PhD student for 2017 start (L. Benini, viva passed over summer).

Funding opportunity: the DTP studentships should be leveraged against funding opportunities. (1000 characters max.)

The one-month-old link to Inductiva should in due course also lead to support from them. At the moment, this is too early, including for a 2022 start. However, the link might very well lead to the prospective PhD student being able to join Inductiva during their PhD for training purposes. In addition, we are already talking about the possibility of jointly applying for possible EU ITN networks with Inductiva as industrial partner. Furthermore, with my new papers on ML/DL now being written, I should be in a good position to submit standard EPSRC-type applications in 2022.

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Disordered quantum systems continue to play a key role in theoretical developments of modern condensed matter physics. The key observation is that quantum interference can lead to suppression of transport – effectively decoupling systems from their environment. This breakdown of the ergodic hypothesis – at the so-called many-body localization transition – leads to regions in phase space which, due to disorder, no longer thermalize. This has profound implications for the

design of possible quantum storage devices. However, most results available at the moment are numerical in nature and based on standard exact diagonalization methods for small system sizes. In this project, we want to use advances in machine learning methods to investigate how to improve these standard methods when applied to disordered systems. In disordered systems, approximate solutions to systems of equations and eigenvalue problems are often good enough to yield meaningful results for the physics of the underlying quantum systems. In the PhD project, we want to develop such new machine/deep learning techniques to improve the description of said disordered systems. The work will be a mix of computational and analytical work, including appropriate high-performance computing strategies.