S10 Artificial Intelligence for Condensed Matter Physics
Inteligencia Artificial en Física de la Materia Condensada (DFMC-GEFES)

13/07 Wednesday afternoon, Aula 1.5 bis

15:30-16:20 Eliska Greplova (TU Delft)
A data-driven perspective on quantum matter

16:20-16:40 Sergio G. Rodrigo (Universidad de Zaragoza)
Design of plasmonic superconducting transition-edge-sensors with neural networks

16:40-17:00 Daniel del Pozo (Universitat de Barcelona)
Transition metals oxidation state determination through Electron Energy-Loss Spectra and Support Vector Machines

17:00-18:00 **Posters and Coffee**

18:00-18:20 Borja Requena (ICFO)
Certificates of quantum many-body properties assisted by machine learning

18:20-18:40 Pablo Serna (Universidad de Murcia)
Machine learning and displacement transformations to locate the many body localization transition

18:40-19:00 Alejandro Jose Uria-Alvarez (Universidad Autonónoma de Madrid)
Deep learning for disordered topological insulators through their entanglement spectrum

19:00-19:20 Juan José García (Universidad Autonónoma de Madrid)
Deep Learning for the modeling and inverse design of radiative heat transfer

Posters:

21 Pedro Moronta (CSIC)
Can random laser networks learn?

22 Miguel Dalmau (Universidad Autónoma de Madrid & CSIC)
Graph convolutional neural networks for accelerating property predictions of small organic molecules

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Design of plasmonic superconducting transition-edge-sensors with neural networks

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We demonstrate the use of neural networks (NN) to improve the design of plasmonic nanostructures. The scattering properties of a plasmonic nanostructure calculated by a slow numerical method is subrogated by a trained NN. The NN results are almost indistinguishable from those calculated with the numerical solver (FDTD method), but up to 10^6 times faster. We illustrate the capabilities of this approach by optimizing a Transition Edge Sensor (TES) to efficiently absorb infrared light. TES are extremely sensitive thermometers made of superconducting metals operating at their transition temperature, where small variations in temperature give rise to a measurable increase in electrical resistance. Coupled to suitable absorbers, they are used as radiation detectors with very good energy resolution in several experiments. TES has been thoroughly investigated for the detection of radiation in the X-ray range. Recently, we purposed a plasmonic TES to work at telecom wavelengths [1]. We designed a high absorbing TES (98% at $\lambda = 1550$ nm) by nanostructuring directly its metal surface, avoiding the use of an extra absorber to reduce the total heat capacity and to simplify the fabrication.

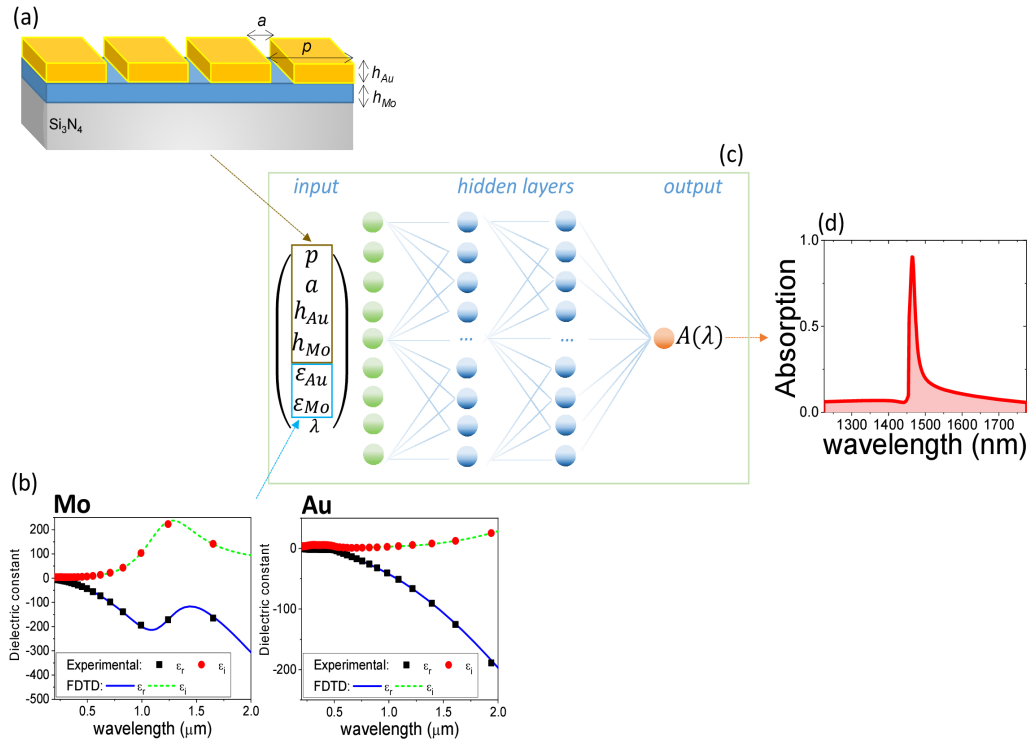

Figure 1. The NN model takes as input: the geometrical parameters of the nanostructure, the dielectric constants of the materials, and the wavelength of light λ. The output layer predicts the absorption at λ.

[1] Sergio G. Rodrigo, Carlos Pobes, Marta Sánchez Casi, Luis Martín-Moreno, and Agustín Camón Lasheras, *Opt. Express* **30**, 12368-12377 (2022)

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Transition metals oxidation state determination through Electron Energy-Loss Spectra and Support Vector Machines

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Electron Energy-Loss Spectroscopy (EELS) is a powerful spectroscopic technique to study locally the composition and properties of materials at the nanoscale, which is carried out in the Scanning and Transmission Electron Microscopes (S/TEM). The recent technological advances in S/TEM devices are leading to higher spatial and energy resolution resulting in an enormous increase of the total amount of data acquired in EELS measurements. Thus, currently this technique offers better energy and spatial resolutions making possible a better nanometric characterization, at the cost of producing large spectral datasets.

The machine learning methods provide a large variety of tools to properly deal with these large amounts of spectral data in an automated manner, at the same time that allow for extracting valuable physical information. A promising machine learning strategy for identifying EELS data is the Support Vector Machine (SVM) [1], in particular the soft-margin SVM, which is a supervised machine learning algorithm allowing the multiclass classification, even with non-linear data, and that can be used as a probabilistic classifier.

The soft-margin SVM has shown promising results identifying the oxidation state in transition metal (TM) oxides, manganese and iron oxides, through the study of their EELS spectra, namely, their white lines (L_3 and L_2) as shown in Figure 1 [2]. The algorithm has been implemented in Python from the library Scikit-learn [3], in particular, the LIBSVM library [4]. It has presented a performance, above 90% classifying the TM oxidation state, even if considering the usual level of noise and additional instrumental energy shifts.

In conclusion, the SVM applied to EEL spectra makes the most of its simplicity (few parameters to optimize) and short computation times to correctly and automatically identify the oxidation state of the transition metals. Furthermore, for large spectral datasets the computing times can even be reduced by implementing the Stochastic Gradient Descend (SDG), which is an iterative method that optimizes, and so, accelerates model training enabling also faster parameter optimization.

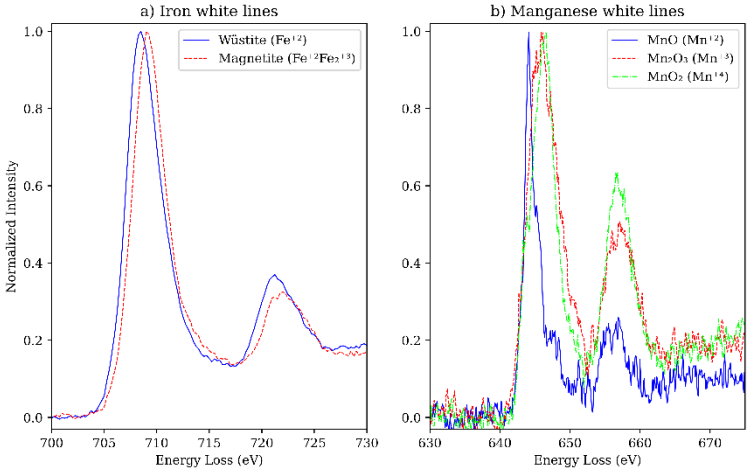

Figure 1. Iron oxides Electron Energy-Loss Spectra: a) Iron white lines for the magnetite (Fe3O4) and wüstite (FeO) oxides, b) Manganese white lines for three manganese oxides.

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[3] F. Pedregosa et al., *Journal of Machine Learning Research* **12**, 2825 (2011).
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Certificates of quantum many-body properties assisted by machine learning

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Computationally intractable tasks are often encountered in physics and optimization. Such tasks usually comprise a cost function to be optimized over a so-called feasible set, which is specified by a set of constraints. This may yield, in general, to difficult and non-convex optimization tasks. A number of standard methods are used to tackle such problems: variational approaches focus on parameterizing a subclass of solutions within the feasible set. In contrast, relaxation techniques have been proposed to approximate it from outside, thus complementing the variational approach to provide ultimate bounds to the global optimal solution.

In this work [1], we propose a novel approach combining the power of relaxation techniques with deep reinforcement learning in order to find the best possible bounds within a limited computational budget. We illustrate the viability of the method in the context of finding the ground state energy of many-body quantum systems, a paradigmatic problem in quantum physics. We benchmark our approach against other classical optimization algorithms such as breadth-first search or Monte-Carlo, and we characterize the effect of transfer learning. We find the latter may be indicative of phase transitions, implementing a completely autonomous approach. Finally, we provide tools to generalize the method to other common applications in the field of quantum information processing.

[1] B. Requena, G. Muñoz-Gil, M. Lewenstein, V. Dunjko, J. Tura, *arXiv:2103.03830* (2021).

Acknowledgements: ICFO group acknowledges support from: ERC AdG NOQIA, Agencia Estatal de Investigación (the R&D project CEX2019-000910-S, funded by MCIN/ AEI/10.13039/501100011033, Plan National FIDEUA PID2019-106901GB-I00, FPI), Fundació Privada Cellex, Fundació Mir-Puig, and from Generalitat de Catalunya (AGAUR Grant No. 2017 SGR 1341, CERCA program). G.M.-G. acknowledges funding from Fundació Obra Social "la Caixa" (LCF-ICFO grant). J. T. thanks the Alexander von Humboldt foundation for support. This project has received funding from the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) – Project number 414325145 in the framework of the Austrian Science Fund (FWF): SFB F7104. This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 899354. This work was supported by the Dutch Research Council (NWO/OCW), as part of the Quantum Software Consortium programme (project number 024.003.037).

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Machine Learning and Displacement transformations to locate the Many Body Localization transition

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The Many-Body localization (MBL) transition [1] is one of the simplest interacting quantum problems, and yet even its precise location in relatively simple models is disputed. The main hurdle is the exponential increase of the size of the Hilbert space with the system size. It imposes constraints to memory and computational time that are very hard to overcome.

Recently, several techniques have been developed to deal with this issue. In particular, the use of unitary displacement transformations [2,3] to obtain eigenstates provides a way to control the approximations that are necessarily made to access large system sizes. With this technique the memory constraint can be overcome but it is compensated with a longer computational time to fully diagonalize the Hamiltonian [4].

We will show how using Machine Learning techniques, namely gradient boosting and deep neural networks, we can exploit the data obtained during the process of diagonalization with displacement transformations to speed up the proccess. The insight from this techniques allow us to classify localized and extended states up to system sizes much larger than what is reported in the literature $L \gg 32$.

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[2] Rademaker L, Ortuño M. *Phys. Rev. Lett.* 116 (2016) 010404. doi:10.1103/PhysRevLett.116.010404

[3] Rademaker L, Ortuño M, Somoza AM. *Annalen der Physik* 529 (2017), 1600322. doi:10.1002/andp.201600322

[4] Serna P, Ortuño M, Somoza AM. *Frontiers in Physics* (2021) 664. doi:10.3389/fphy.2021.767001

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Deep learning for disordered topological insulators through their entanglement spectrum

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Calculation of topological invariants for crystalline systems is well understood in reciprocal space, allowing for the topological classification of a wide spectrum of materials [1, 2]. While working in the reciprocal space may still be possible for disordered materials, computations will become too expensive due to the mandatory increase in cell size. On top of that, the most popular techniques such as the Wilson loop [3] are only well-defined in insulating materials, generally defined as systems with fully occupied bands or partially occupied ones, but separated from the rest by a gap across the whole Brillouin zone.

In this work [4], we present a technique based on the entanglement spectrum, which can be used to identify the hidden topology of systems [5] without translational invariance. By training a neural network to distinguish between trivial and topological phases using the entanglement spectrum obtained from crystalline or weakly disordered phases, we can predict the topological phase diagram for generic disordered systems. This approach becomes particularly useful for gapless systems, while providing a computational speed-up compared to the commonly used Wilson loop technique for gapful situations. Our methodology is illustrated in two-dimensional models based on the Wilson-Dirac lattice Hamiltonian.

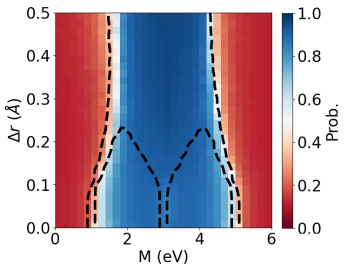

Figure 1. Topological phase diagram as predicted by the neural network. Black lines correspond to gap contour lines for 0.1 eV.

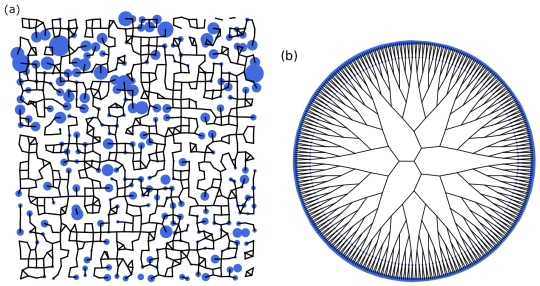

Figure 2. Edge state in (a) an amorphous lattice and (b) in the Bethe lattice.

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Deep Learning for the modeling and inverse design of radiative heat transfer

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Deep learning is having a tremendous impact in many areas of computer science and engineering. Motivated by this success, deep neural networks are attracting an increasing attention in many other disciplines, including physical sciences. In this work [1], we show that artificial neural networks can be successfully used in the theoretical modeling and analysis of a variety of radiative heat transfer phenomena and devices. By using a set of custom-designed numerical methods able to efficiently generate the required training datasets, we demonstrate this approach in the context of three very different problems, namely, *(i)* near-field radiative heat transfer between multilayer systems that form hyperbolic metamaterials (figure 1), *(ii)* passive radiate cooling in photonic-crystal slab structures (figure 2), and *(iii)* thermal emission of subwavelength objects. Despite their fundamental differences in nature, in all three cases we show that simple neural network architectures trained with datasets of moderate size can be used as fast and accurate surrogates for doing numerical simulations, as well as engines for solving inverse design and optimization in the context of radiative heat transfer. Overall, our work shows that deep learning and artificial neural networks provide a valuable and versatile toolkit for advancing the field of thermal radiation.

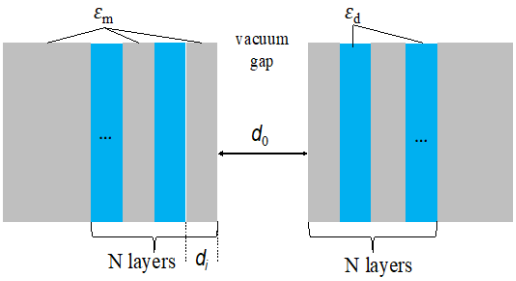

Figure 1. Sketch of two identical multilayer systems separated by vacuum and composed of layers of width d_i alternating between a Drude metal (grey) with permittivity ε_m and a dielectric (blue) with permittivity ε_d. Inspired by the design from [2].

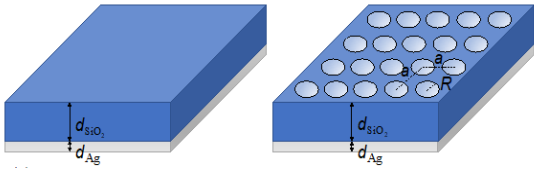

Figure 2. Left: Schematics of a silica mirror used in [3] as a passive radiative cooler, consisting of a SiO_2 slab of thickness d_{SiO2} and a silver thin film of thickness d_{Ag}. Right: same mirror, but with a periodic array of holes in the silica layer, with radius R and lattice parameter a.

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Acknowledgements: J.J.G.E. was supported by the Spanish Ministry of Science and Innovation through a FPU grant (FPU19/05281). J.B.A. acknowledges financial support from Ministerio de Ciencia, Innovación y Universidades (RTI2018-098452-B-I00). J.C.C. acknowledges funding from the Spanish Ministry of Science and Innovation (PID2020-114880GB-I00).

Can random laser networks learn?

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The ever-increasing energy demand of conventional Artificial Intelligence (AI) hardware calls for disruptive approaches in which the training process can be less power-hungry and less environmentally harmful. Reservoir computing and extreme machine learning are two particularly appealing approaches that, by exploiting the natural dynamics of input-driven randomly connected neural networks, feature minimal energy requirements. Remarkably, photonics is emerging as a natural testbed to implement both reservoir computing and extreme machine learning that can represent realistic alternatives to the ubiquitous von Neumann architecture [1].

In this preliminary work, we discuss how a network of coupled random lasers (RLs) can be tailored to realize a novel platform for reservoir computing and extreme machine learning. We generalize to complex networks our recent experimental and numerical work investigating the coupling of few RLs based on a pumped gain-medium strip connecting two rough mirrors [2]. We particularly focus on a system based on three-resonator arranged in a Z-shaped configuration and show how the coupling of lasers modes between non-neighbouring resonators via a linking resonator can indeed provide the basis for a whole new paradigm in reservoir computing.

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Graph convolutional neural networks for accelerating property predictions of small organic molecules

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In recent years graph neural networks (GNNs), a branch of deep learning exploiting graph structures, have found a very wide range of applications across industry and science [1]. GNNs offer significant potential in the context of property prediction of solids [2] and molecules [3], for which graph features (nodes and edges) allow for a natural self-contained and accurate description of the system.

In this work, we demonstrate an efficient implementation of graph convolutional neural networks for accelerating the property predictions of small molecules made up of C, H, O, N, F (of up to nine atoms not counting H). Using an existing database containing quantum chemical calculations of 134,000 molecules [4], we show how a GNN architecture consisting of a small number of GNN convolutional layers, followed by a densely connected neural network enables an efficient prediction of the internal energy of the considered class of molecules (see Fig. 1). In our approach, each graph node represents an atom, and the corresponding edges include information about atom distances, bond angles and, optionally, dihedral angles.

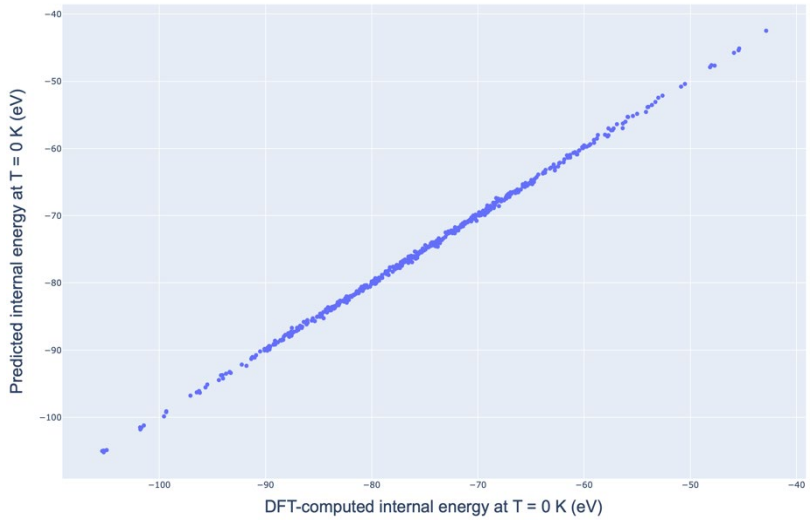

Figure 1. Comparison between the predicted internal energy at T=0K predicted by the proposed GCNN implementation and that calculated with a density-functional-theory approach. Each blue circle in the figure represents the results of one of the molecules included in a test set not included in the training process of the proposed algorithm.

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