AFRL-AFOSR-VA-TR-2023-0199

Probing the Quantum-Classical Transition with Bayes-Enhanced Scanning Gate Microscopy

Carlo da Cunha
UNIVERSIDADE FEDERAL DO RIO GRANDE DO SUL
AV. PAULO GAMA 110
PORTO ALEGRE, RS, 90040-060
BRA

11/22/2022
Final Technical Report

Air Force Research Laboratory
Air Force Office of Scientific Research
Arlington, Virginia 22203
Air Force Materiel Command

REPORT DOCUMENTATION PAGE

PLEASE DO NOT RETURN YOUR FORM TO THE ABOVE ORGANIZATION.

1. REPORT DATE	2. REPORT TYPE	3. DATES COVERED	
20221122	Final	START DATE 20200915	END DATE 20220914

4. TITLE AND SUBTITLE
Probing the Quantum-Classical Transition with Bayes-Enhanced Scanning Gate Microscopy

5a. CONTRACT NUMBER	5b. GRANT NUMBER	5c. PROGRAM ELEMENT NUMBER
	FA9550-20-1-0377	
5d. PROJECT NUMBER	**5e. TASK NUMBER**	**5f. WORK UNIT NUMBER**

6. AUTHOR(S)
Carlo da Cunha

7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)
UNIVERSIDADE FEDERAL DO RIO GRANDE DO SUL
AV. PAULO GAMA 110
PORTO ALEGRE, RS 90040-060
BRA

8. PERFORMING ORGANIZATION REPORT NUMBER

9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES)	10. SPONSOR/MONITOR'S ACRONYM(S)	11. SPONSOR/MONITOR'S REPORT NUMBER(S)
Air Force Office of Scientific Research 875 N. Randolph St. Room 3112 Arlington, VA 22203	AFRL/AFOSR IOS	AFRL-AFOSR-VA-TR-2023-0199

12. DISTRIBUTION/AVAILABILITY STATEMENT
A Distribution Unlimited: PB Public Release

13. SUPPLEMENTARY NOTES

14. ABSTRACT
The principal goal of this project was to devise techniques to obtain information from scanning gate microscopy images. For this, we have created numerical packages to compute non-equilibrium Green's functions (NEGF) and implemented a cellular neural network architecture to estimate the potential given a local density of states. We report the development of two successful approaches that can be used in quantum constrictions to estimate the alloy potential as well as the formation of charge puddles.

15. SUBJECT TERMS

16. SECURITY CLASSIFICATION OF:			17. LIMITATION OF ABSTRACT	18. NUMBER OF PAGES
a. REPORT U	b. ABSTRACT U	c. THIS PAGE U	SAR	9

19a. NAME OF RESPONSIBLE PERSON	19b. PHONE NUMBER *(Include area code)*
CHRISTOPHER CARSON	000-0000

Report Coversheet

Award Number

FA9550-20-1-0377

Report Type

Final Performance Report

Reporting Periods

Start 15 SEP 2020 – End 14 SEP 2022

Distribution Statement

Approved For Public Release

Program Officer Name

Dr. Badford Barrett

Principal Investigator Name

Dr. Carlo Requiao da Cunha

Project Title

Probing the Quantum-Classical Transition with Bayes-Enhanced Scanning Gate Microscopy

ABSTRACT

The principal goal of this project was to devise techniques to obtain information from scanning gate microscopy images. For this, we have created numerical packages to compute non-equilibrium Green's functions (NEGF) and implemented a cellular neural network architecture to estimate the potential given a local density of states. We report the development of two successful approaches that can be used in quantum constrictions to estimate the alloy potential as well as the formation of charge puddles.

Chapter 1

Accomplishments

Phase-sensitive devices such as quantum point contacts (QPC) and quantum dots (QD) may lead to the development of electronic devices with potential applications in high-performance/quantum computing. Obtaining graphical information about the structure and operation of these devices is of utmost importance to aid appropriate designs.

1.1 Research Objectives

The current project aimed at developing a Bayes-enhanced strategy to acquire information from images obtained from Scanning Gate Microscopy (SGM) [1]. This is a technique where a charged scanning probe rasters the surface of a quantum-effect device while changes in conductance are monitored. A map of conductance variations is then produced and, under some strict conditions, this is connected to the local density of states of the device.

According to first-order perturbation theory:

$$\Delta\mathcal{E}_n \approx V_0|\varphi_n(\mathbf{r})|^2, \tag{1.1}$$

where $\Delta\mathcal{E}_n$ is the energy shift of the n^{th} energy level, V_0 is the tip potential, and $\varphi(\mathbf{r})$ is the wavefunction evaluated at the tip position $\mathbf{r}$.

At low temperatures, the transport happens at the surface of the Fermi sea. Therefore, the change of conductance is given by:

$$\Delta G(\mathbf{r}) \approx \frac{\partial G}{\partial \mathcal{E}_F}\Delta\mathcal{E}_n, \tag{1.2}$$

where G is the conductance and $\mathcal{E}_F$ is the Fermi energy.

The obtained images, though, are typically difficult to interpret and susceptive to decoherence effects. Therefore, the ultimate goal of this project was to develop a strategy to estimate the potential of the electronic device that contributes to the formation of observed patterns in the conductance map.

1.2 Accomplishment Details

We succeeded in developing not one but several techniques to estimate the background potential of phase-sensitive devices using a collection of machine learning procedures. The most successful approaches were obtained using cellular neural networks and a quasi-model-free approach using a

swarming algorithm. We were able to recreate potentials that produce a local density of state images at least 72 % correlated with the experimental results. In both cases, we observed an increase in the granularity of the potential as our prototypical quantum point contact was squeezed. Furthermore, our approaches allow one to estimate not only the static alloy potential but also the formation of charge puddles in these devices.

1.3 Dissemination

A book was published comparing quantum systems with economic systems [7]. With the scaling of the CMOS technology reaching its limits, studying novel devices such as the phase-sensitive devices studied in this project becomes eminent. On the other hand, exploring novel architectures may also lead to the development of solutions to this scaling. Economic and biological systems, for instance, are capable of solving tough NP problems with energy efficiencies much higher than those of current supercomputers. This book is the first step in trying to borrow some ideas from these other sciences for the development of highly efficient electronic systems. This reaches a wide audience and introduces many physical concepts to communities other than that of physicists.

C. R. da Cunha, "Introduction to Econophysics: Contemporary Approaches with Python Simulatuions" 1st ed. (2021) CRC Press - Boca Raton, FL - ISBN: 978-0367648459.

It is currently difficult to find a rigorous treatment of machine learning algorithms as most of the published material is superficial and deals only with applications. In another book that is currently being written, we explore regression models, clustering algorithms, and neural networks with mathematical rigor. The book will be published in 2023 and is targeted to individuals of many disciplines including engineering, computer science, and physics.

C. R. da Cunha, "Machine Learning for the Physical Sciences: Fundamentals and Prototyping with Julia" 1st ed. (2023) CRC Press - Boca Raton, FL.

1.3.1 Journal Papers

We have prepared three scientific papers with the main results of this research:

C. R. da Cunha, N. Aoki, D. K. Ferry, A. Velasquez, and Y. Zhang, "An investigation of the background potential in quantum constrictions using scanning gate microscopy and a swarming algorithm" Under revision in *Physica A* (2022).

C. R. da Cunha, N. Aoki, D. K. Ferry, and Y. -C. Lai,"A method for finding the background potential of quantum devices from scanning gate microscopy data using machine learning", *Mach. Learn. Sci. Tech.* **3-2** (2022) 025013.

R. Borrasca Neto, B. J. Becker, and C. R. da Cunha, "Extending spin market models to realistic scenarios", *Int. J. Mod. Phys. C* **33-08** (2022) 2250101.

The first paper was produced in collaboration with Profs. David Ferry and Yu Zhangfrom Arizona State University, Prof. Nobuyuki Aoki from Chiba University in Japan, and Prof. Alvaro Velasquez from the University of Colorado Boulder (previously at AFRL - Information Directory).

This is a paper where we discuss the use of a quasi-model-free approach to estimate the background potential of quantum structures.

The second one was produced in collaboration with Professors David Ferry and Ying-Cheng Lai from Arizona State University and Professor Nobuyuki Aoki from Chiba University in Japan. It contains the main results of estimating the potential from SGM images.

In the third paper, we expand a metastable spin model (the Bornhold model) to realistic complex network topologies and study the behavior of the model as a function of topological parameters. We found that this extended spin model is capable of reproducing many stylized facts found in the financial sector if the topology of the network is properly adjusted.

1.3.2 Conferences

Due to the pandemic, we were only able to submit articles for conferences in 2022/2023:

C. R. da Cunha, "An investigation of the disorder potential of quantum point contacts via scanning gate microscopy and machine learning" - Submitted to the March Meeting of the American Physical Society (2023) Las Vegas, NV.

C. R. da Cunha, N. Aoki, D. K. Ferry, "Inferring the self-consistent background potential of quantum constrictions via scanning gate microscopy and machine learning" Workshop on Innovative Nanoscale Devices and Systems (2022) Lihue, HI - Accepted.

These articles condense all our findings obtained from this research. The first one is considered for a presentation at the March Meeting of the American Physical Society in Las Vegas, NV, whereas the other one was accepted for a conference in Lihue, HI in December 2022.

1.3.3 Miscellaneous

All results are published on my personal webpage: https://ac.nau.edu/∼cc3682. All developed codes were made publicly available on https://github.com/StxGuy/. This includes:

1. Econophysics: Set of codes for statistical mechanics that draws parallels between economics and physical systems;
2. MachineLearning: Set of codes for unsupervised, supervised, neuronal inspired, and reinforcement learning;
3. NobleNeuron: Library for feedforward neural networks;
4. TenaciousTensors: Library for handling multidimensional arrays and tensors;
5. GreenCheetah: Numerical package for non-equilibrium Green's functions.

Chapter 2

Impacts

2.1 Development of the principal and other disciplines

Two main developments are likely to cause a big impact on the base of knowledge. First, we developed a method for estimating the background potential of quantum-effect devices and this may be used by several groups to qualify the impurity level of novel quantum materials and improve the performance of devices. Furthermore, we created a machine learning algorithm that does not depend on any specific neural network model or a specific training set. This can be used by several researchers to solve reverse problems in quantum mechanics that are typically difficult to tackle using contemporary approaches. This may lead to the design of quantum-effect devices for specific purposes.

Our main results were published in Machine Learning: Science and Technology, which has an outstanding impact of 6.013. Also, we have results being peer reviewed at Physica A which has an impact factor of 3.778. These results not only are useful for physicists but may also be interesting to computer scientists and engineers interested in device physics and machine learning.

2.2 Human resources

During the development of this research, three graduate students coming from families with economic difficulties worked on this project. All of them are now employed and one of them was recruited by a Spanish company. The principal investigator was offered a professor position at the Northern Arizona University.

2.3 Impact on teaching

The results obtained in this research lead to the development of two books. One of them is already being used as the main text in courses about Econophysics at the Universidade Federal do Rio Grande do Sul in southern Brazil.

Chapter 3

Changes

3.1 Changes in Approach

To make numerical calculations, two packages were written in Fortran. One to compute NEGF and another to train CNN. Although they were used to obtain results that were published, maintenance and expansion of these packages are difficult. Therefore, we translated our codes into the Julia programming language. Computation speeds were comparable, but the codes are much more legible and easier to expand. Julia became the official language of the group.

To make calculations, two main Fortran packages were created, one for computing Green's functions in quantum systems and another for training and inferring from Cellular Neural Networks. Another package using a swarming algorithm to estimate the background potential was written in Julia.

To obtain information about the device based on the SGM data, we experimented with some machine learning algorithms. The original idea was to use generative adversarial networks to reconstruct and enhance the resolution of such microscopy images, but we ended up using a cellular neural network (CNN) structure [3]. The original idea of using Bayes inference was discarded due to an intractable number of parameters. Moreover, compared to a generative-adversarial network (GAN) [4], the CNN showed results much closer to the theoretical data obtained using NEGF.

Although CNN produced high-quality results that were published, these results were bounded by the training set. Therefore, by the end of the reporting period, we developed an algorithm that does not depend on any neural network model but uses a swarming approach where the estimated potential is progressively improved as quantified by the correlation between the density-of-states computed by NEGF and the experimental data.

3.2 Problems or Delays

The biggest problem that happened during the reporting period was the COVID pandemic. Many countries were closed to Brazilian citizens, and most of the important conferences were cancelled. As a result, we were only able to submit articles for conferences that happen by 2022/2023. Moreover, since the university was closed during the whole performing period, it was extremely difficult to recruit graduate students to work on this project.

3.3 Expenditure Impacts

Nothing to report.

Chapter 4

Technical Updates

To execute this project, it was first necessary to code numerical packages for calculating the quantum properties of phase-sensitive devices. For this, we used non-equilibrium Green's functions (NEGF) [2]. These calculations are used as theoretical estimates of the behavior of quantum-effect devices. They were coded in Fortran during the first eight months of the project.

Consequently, another package for cellular neural networks (CNN) was created to infer the background potential from SGM. Instead of using popular packages such as Tensorflow and Pytorch, we created our package. This is because these packages are mostly developed to deal with generic problems in Python. On the other hand, the amount of data that we must use to handle SGM is huge and speed becomes a limiting factor. Therefore, we opted to create dedicated packages in Fortran using parallel processing in a Graphical Processing Unit (GPU). This took us eight months of coding.

Some results using a modified CNN were obtained to infer the background potential of QPC. This took us six months of tuning the packages, obtaining theoretical data using NEGF, and training the CNN. A paper with the main results was published [5]. A concomitant strategy using spin automata was pursued as an idea to produce high-speed devices [6].

More recently, we developed a quasi-model-free algorithm to estimate the background potential of phase-sensitive devices without relying on any particular neural network model. A paper with these results is under peer review at Physica A.

4.1 Green's Functions

To train the network, a Fortran package for calculating Green's function was created. In the computation, the device is split into a set of vertical independent segments, and the Hamiltonian for each slice is computed as:

$$G^0_{n,n}(\mathcal{E}) = \left[(\mathcal{E} + i\eta)\,\mathbf{I} - \mathbf{H}_n\right]^{-1}, \tag{4.1}$$

where $\mathcal{E}$ is the energy at which the calculation is performed, n is an index for the slice, η is a constant that approaches zero, and $\mathbf{H}_n$ is the Hamiltonian for the slice.

Slices are connected to find a Green's function using Dyson's equation:

$$G_{a,b} = G^0_{ab} + \sum_{m,n} G^0_{a,m} V_{m,n} G_{n,b}, \tag{4.2}$$

where G^0 is the unperturbed Green's function, and $V_{a,b}$ is the coupling matrix between segments a and b.

The local density of states (LDOS) is given by:

$$D_n = -\frac{1}{\pi}\mathrm{Im}\{G_{n,n}\} \tag{4.3}$$

and the transmission between two slices is given by:

$$t = \mathrm{Tr}\left[\Gamma_L G_{LR} \Gamma_R G_{LR}^{\dagger}\right], \tag{4.4}$$

where

$$\Gamma_{L,R} = i\left[\Sigma_{L,R} - \Sigma_{L,R}^{\dagger}\right] \tag{4.5}$$

and Σ is the self-energy of each lead.

4.2 Cellular Networks

To infer the potential from SGM images, we modified the standard cellular neural network architecture. This is a dynamical system whose state evolves by:

$$\frac{dX_{ij}(t)}{dt} = -X_{ij}(t) + \sum_{(k,l)\in\mathcal{N}_{ij}} A_{ijkl} Y_{kl}(t) + \sum_{(k,l)\in\mathcal{N}_{ij}} B_{ijkl} U_{kl}(t) + 1, \tag{4.6}$$

where $\mathcal{N}_{ij}$ is the Moore neighborhood around the cell (i, j) and the tensors $\mathbf{A}$ and $\mathbf{B}$ are known as *cloning templates*.

Instead of a simple saturation as initially proposed for the CNN, we used a hyperbolic tangent activation. Furthermore, the training of the network was performed considering an L_2 error given concerning the expected potential. A gradient descent approach was used in combination with the Euler method to obtain new values of the cloning template.

For the LDOS-Potential pairs produced using Green's function approach, we obtained a minimum L_2 error of around $\pm 7\%$.

Bibliography

[1] For a review, see: N. Aoki, C. R. da Cunha, R. Akis, D. K. Ferry, and Y. Ochiai, "Scanning gate imaging of a disordered quantum point contact", *J. Phys.: Cond. Matt.* **26**-19 (2014) 193202.

[2] D. K. Ferry, S. M. Goodnick, and J. Bird, "Transport in nanostructures" 2nd (2009) Cambridge University Press, Cambridge, UK.

[3] L. O. Chua and L. Yang, "Cellular neural networks", *IEEE Trans. Circ. Sys.* **35** (1988) 1257.

[4] I. Goodfewllow, J. Pouget-Abadie, M. Mirza, B. Xu, D. Warde-Farley, S. Ozair, A. Courville, Y. Bengio, "Generative Adversarial Nets" *Proc. Conf. Neural Inf. Proc. Sys.* (2014) 2672–2680.

[5] C. R. da Cunha, N. Aoki, D. K. Ferry, and Y.-C. Lai, "A method for finding the background porential of quantum devices from scanning gate microscopy using machine learning" *Mach. Learn. Sci. Tech.* **3** (2022) 025013.

[6] R. Borrasca Neto, B. J. Becker, and C. R. da Cunha, "Extending spin market models to realistic scenarios" *Int. J. Mod. Phys. C* **33-08** (2022) 2250101.

[7] C. R. da Cunha, "Introduction to Econophysics: contemporary approaches with Python simulations" (2021) CRC Press, Boca Raton, Fl.