ERC Advanced Grant 2018
Research proposal [Part B1]
(Part B1 is evaluated both in Step 1 and Step 2
Part B2 is evaluated in Step 2 only)

Quantum Simulation in Artificial lattices

QUASAL

Cover Page:
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The radical failure of conventional computers to tackle the many body problem leaves our understanding of many fascinating scientific questions, such as the origin of high temperature superconductivity, in the hands of a strike of inspiration. Whereas other big problems have been solved like that, it would be great to have an efficient way simulate quantum matter. It is now self-evident that quantum simulations hold the promise of handling us the resources to figure out the many-body problem, something that will radically change the way we do condensed matter physics. Now the challenge is to design quantum simulators. QUASAL addresses this challenge and, through thorough realistic modelling, provides a roadmap to implement Analog Quantum Simulations of flagship model Hamiltonians on artificial lattices based on three different solid state platforms:
* Functionalized graphene bilayers, to simulate the Hubbard model
* Nanoengineered spin arrays, fabricated and probed with scanning tunnelling microscopes, to simulate short range spin models
* Laser driven transition metal dichalcogenides, that permit laser controlled interactions between localized spins diluted in the host.
Using a combination of density functional theory calculations, exact diagonalizations, density matrix renormalization group, machine learning and quantum digital simulation, this proposal targets three goals: 1) to demonstrate how the platforms above simulate critically important model Hamiltonians, and to predict the model energy scales. 2) To design experiments that permit to simulate non-trivial physics, such as fractionalization in low dimensional spin liquids. 3) To determine protocols of validation of the quantum simulations. This proposal paves the way to a radically new way to understand nature, that blurs the difference between experiments and computation, and that circumvents the exponential wall problem which hampers classical modelling of quantum systems.

Section a: ***Extended Synopsis of the scientific proposal (max. 5 pages)***

In a nutshell: Led by Principal Investigator, the project QUASAL will put together a top-class team of theoretical quantum physicists. The goal: to make quantum simulation of many-body Hamiltonians possible. The strategy: to provide a roadmap for the fabrication and benchmarking of new platforms for Analog Quantum Simulation of the Hubbard and Ising and Heisenberg models, taking advantage of recent breakthroughs in atomic manipulation and the discovery of certain 2D materials.

1. The problem: the exponential wall

The formulation of quantum mechanics permits an extremely accurate description of a few simple systems, such as the hydrogen atoms, and provides a platform for an approximate description of a variety of phenomena involving many interacting electrons and atoms. For the purpose of solving the Schrödinger equation exactly, "a large number" can be as small as 3 electrons. Whereas approximations do a fair or even great job in many cases, there are some outstanding problems that we have not been able to solve yet. This includes, for instance, understanding the origin of high temperature superconductivity in correlated electron materials and the lack of accurate methods to address some extremely relevant quantum chemistry problems, such as the workings of natural biomolecules that solve the nitrogen fixation problem in an energy efficient manner, or the photovoltaic energy conversion.

The failure of computational "brute force" solutions for the Schrödinger equation, based on classical computers, is linked to so called exponential wall problem[KOH99]: the number of computing resources needed to solve the Schrödinger equation of a system with N degrees of freedom scales exponentially. For instance, if we want to write up just 1 quantum state describing N spin S=1/2 spins, say N=300, we need to store 2^N complex numbers somewhere. The problem is that there are only 2^{265} atoms in the universe. Therefore, exact solutions can only handled for very small quantum chemistry problems, such as the H_2 molecule, or some specific model Hamiltonians, most of them in one dimension. If giving up is not an option, we need to have a radically different approach in order to find a systematic solution to the quantum many body problem.

2. The solution: quantum simulations

The way around the exponential wall can be found in the so called quantum simulators, a notion put forward by Feynman[FEY82]. After more than 35 years of work, it is now self-evident that quantum systems store quantum information much more efficiently than classical resources. The challenge is to design and put to work quantum machines that carry out computations. In all instances, this requires the fabrication of a network of quantum objects whose interconnections are controlled externally. The artificial quantum lattices studied in this project are one example of such quantum machines.

Quantum simulations come in two very different flavours: Digital and Analog [GEO14]. Digital quantum simulations run on general purpose quantum computers. They rely on extremely elegant algorithms, such as the quantum Fourier Transform and quantum phase estimation algorithms, and hold the promise of calculating the ground state energy, and other important observables, of most of the Hamiltonians that condensed matter and quantum chemistry deal with. In order to simulate a fermion problem with N single particle states, they only need O(N) qubits. The major requirement, that will keep digital quantum simulation at bay for a few years, comes from the number of gate operations, necessary to run the algorithm: in the range of hundreds for a chemically simple system such as H_2. Due to decoherence and noise in the gate operations, state of the art computers can only tackle trivial problems at this point.

The current challenges for Digital Quantum Simulation motivate the focus on the so called Analog Quantum simulators. These are : "*any physical quantum system precisely prepared or manipulated in a way aimed at learning interesting properties of (..)quantum systems*", as defined by Eisert et al. (in chapter 4 in [ACI8]). The main goal of QUASAL it to propose new strategies for Analog Quantum simulation of two types of very important Hamiltonians, the Hubbard model, that is believed to hold the key to understand high temperature superconductivity, and the Ising and Heisenberg spin models, that account for a large number of non-trivial many-body phenomena, such as quantum phase transitions, topological order and fractionalization.

The requirements to build Analog Quantum Simulators are less demanding than those needed to have full fledge universal quantum computers. Some physical platforms, such as cold atoms [BLO12] and trapped ions[BRI12], have been used to simulate the Hubbard model and spin model Hamiltonians. However, they have some severe problems. For instance, cold-atoms can only simulate the Fermi Hubbard model at temperatures comparable to the relevant energy scales. Therefore, cold-atom simulators can not address

properly all the interesting emergent phenomena of Hubbard models, such as correlated superconductivity and spin-charge separation. On the other hand, trapped ions are a wonderful platform to handle quantum information, but when it comes to Analog Quantum Simulation, they can only handle spin models with long-range interactions, leaving out spin-models that are relevant for real materials. Therefore, there is an urgent need to find alternative strategies for quantum simulation of these important model Hamiltonians.

3 Quantum simulations with Artificial Lattices: objectives

The approach of this project is to explore three different solid state platforms that have a great potential to work as Analog Quantum simulators. In all of them I exploit recent breakthroughs in atomic manipulation and probing as well as in newly discovered materials to design quantum simulators that can be operated with state of the art technologies. Thus, the objectives of QUASAL are:

Objective 1: **To design a platform for analog quantum simulation of Hubbard model that permits to explore a wide range of lattices, filling factors and temperatures.** For this matter I propose to use graphene bilayers with an ordered array of sp^3 defects that introduce localized electronic states within the gap. This permits the simulation of the Hubbard model in a variety of artificial lattices with tunable on-site Coulomb repulsion, hopping energies and filling factors, in the strong quantum degenerate limit.

Objective 2: To design a platform for analog simulation of spin systems with short range interactions, based on engineered adatom arrays on surfaces. Here I propose to take advantage of arrays of magnetic atoms nano-engineered on surfaces using scanning tunneling microscopes (STM), as a platform for AQS of spin Hamiltonians. The focus will be placed on the simulation of quantum disordered phases such as spin liquids in 1D and 2D. This should permit a radically new way to explore spin liquids with artificial lattices.

Objective 3: To find an efficient system to implement time-controlled laser induced exchange interactions between local spins in a semiconductor. Optically induced exchange interactions (OEI) were proposed [PIER02] as a resource to switch on and off exchange interactions between distant local spins using laser pulses. The goal here is to carry out a systematic study of the right combination of host material and local spins to make this happen experimentally. For the host semiconductor I will exploit the very suitable optical properties of two dimensional transition metal dichalcogenides, that include very large Rabi coupling [LIU15], and very large excitonic binding energy, to enhance the magnitude and the range of the OEI.

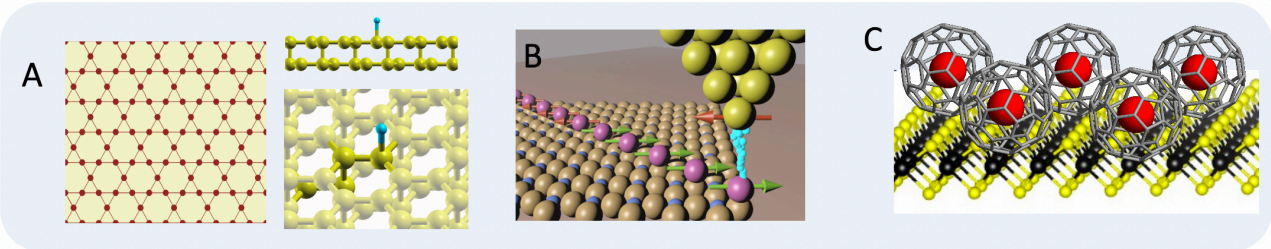

***Figure 1 Artificial quantum lattices**. **A**: Kagome lattice of localized electron states created around carbon sites passivated with atomic hydrogen in Graphene bilayer **B:** a chain of magnetic atoms on a metallic surface, probed and positioned with a STM.. **C** Array of paramagnetic centers ($N@C_{60}$) adsorbed on a transition metal dichalcogenides. Exchange interactions are induced by subgap laser.*

As I argue below, and in B2, the choice of these three quantum simulation platforms are motivated by the following common points:

- They are feasible with state of the art technology, and due to recent breakthroughs, it is now possible to explore their potential for Analog Quantum Simulation
- They will be able to bring a disruptive solution to several outstanding problems in condensed matter
- I have been doing research, both theory only and hand in hand with some of the leading experimental groups in the world, on these material systems.

4. Analog Quantum simulation of the Hubbard model

The Hubbard model is the most important Hamiltonian in the study of correlated electron systems. Its exact solution is only known in one dimension [LIE68] and can be found numerically for clusters with a small number of sites. Out of that, we need to content ourselves with approximations. Whether or not the Hubbard model describes superconductivity in slightly doped Mott insulators [AND97] is one of the central open questions in condensed matter, and out of reach of conventional computation.

Ultracold atoms confined in optical lattices can be used to carry out quantum simulations of the Fermi Hubbard model [COC16] with thousand of fermions. However, the relevant energy scales that settle interactions are of the same order than the temperature of the system. Therefore, these simulations can not explore the region where the most interesting physics is expected to occur. Solid state platforms, such as quantum dots, can go around this problem, but so far quantum simulations have been restricted to a very small number of sites. Therefore, currently there is no efficient platform to simulate the Hubbard model in a large enough simulation cell and at with temperatures much smaller than the relevant energy scales.

Here I propose a radically new approach that takes advantage of several relatively recent discoveries. First, the fact that a widely tunable band-gap, of up to 250 meV, can be opened in graphene bilayer by application of an off-plane electric field [ZHA09]. Second, the theoretical prediction that chemisorption of atomic hydrogen in graphene bilayer induces a localized state that hosts single electron with energy inside the gap, and whose wave function is controlled electrically (see [NIL07]). Third, and crucially important, the recent experimental demonstration [GON16] of chemisorption of atomic hydrogen in graphene, controlled with atomic scale precision using a scanning tunnelling microscope (STM) (see Figure 2).

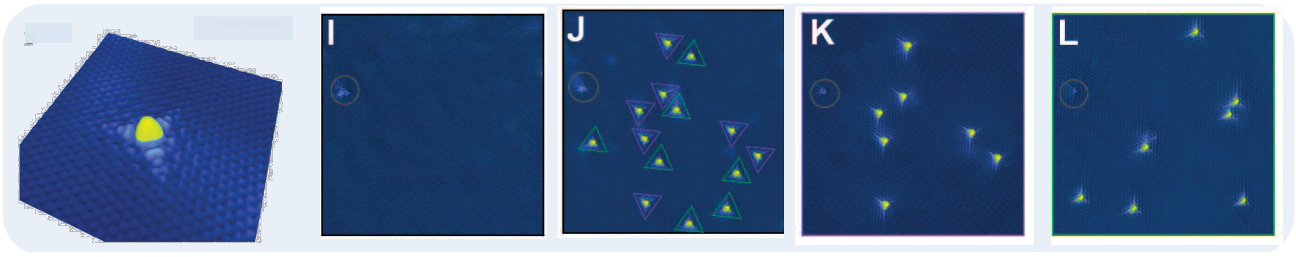

Figure 2 Atomic scale manipulation of Hydrogen on graphene, taken from *[GON16]. **A**: STM scan of a single hydrogen atom on graphene (7x7 nm^2).* **I-J,K,J**: *4 steps of a manipulation sequence, all in the same region of (28x28 nm^2).* ***I**: Pristine area (notice a point defect).* **J** *14 hydrogen atoms are placed, equally shared by the 2 sublattices.* ***K** and L Only atoms of 1 sublattice are kept on place.*

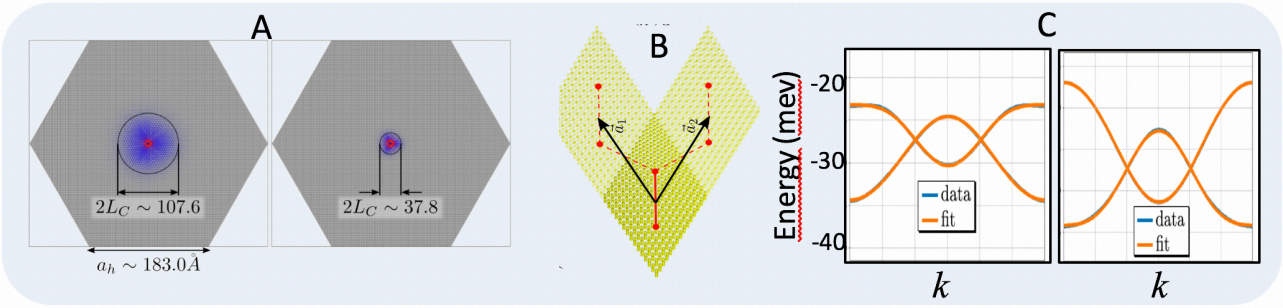

Figure 3: **Electric control of hopping in Hubbard model simulator. A.** *A map of the wave function for a single sp^3, for two different values of the electric field.* **B** *The unit cell of a graphene bilayer functionalized with an array of sp^3 defects, 8.4nm apart, that form a honeycomb pattern.* **C.** *In-gap bands, corresponding to B, for 2 different values of the electric field (blue) fitted to a simple tight-binding model (orange).*

A graphene bilayer functionalized with hydrogen atoms hosts an array of localized states with one electron each. This is the essence of the Hubbard model. The overlap between these states, and thereby the hopping energy (*t*) between them, is determined by two tunable parameters: 1) the separation between defects, that can be controlled with atomic precision [GON16] 2) the size of the band-gap, that depends on the applied field. Our preliminary simulations for a honeycomb array of hydrogen dopants, separated by 8.4nm , show that the in-gap spectrum has the standard dispersion of graphene, with a much narrower bandwidth in the range of 20 meV and, more importantly it can be tuned electrically. The extension of the states also controls the other important energy scale of the Hubbard model, the Coulomb energy overhead (*U*) necessary to add a second electron in a given state. Our preliminary calculations [GAR18] show that *U* can be as high as 10 meV. The hopping energy can be as small as necessary, by increasing the separation between hydrogens. Finally, using a dual gate [TAY10] , the electron density and the gap can be controlled independently. Therefore, this platform can simulate the Hubbard model in a variety of 0D, 1D and 2D arrays, with tunable energy scales *(t,U)* in the range of 1 meV , and tunable filling factor.

This project will focus on a realistic modelling of how graphene bilayer functionalized with hydrogen and other *sp*^{3} defects maps to a Hubbard model, and how transport experiments, both in-plane and with STM, can

provide information about the spectral function of the Hubbard model. I will also address protocols to validate the simulations, using the known solutions in 1D, so that we can trust the simulation of 2D systems, for which independent validations are not possible.

5. Analog Quantum simulation of short-range spin models

Ising and Heisenberg spin model Hamiltonians play a central role in many branches of condensed matter physics, including quantum magnetism. Their exact solutions, in one dimension, describe states that do not order even at zero temperature due to quantum fluctuations. These are the so called spin liquids. According to theory, they feature topological order, fractional excitations (spinons, anyons), fractional edge states [HAL18]. In 1D, both exactly solved models and the density matrix renormalization group (DMRG) numerical method [WHI92] permit an efficient modelling of these phenomena. In contrast, the simulation of quantum spin liquids in 2D is much more challenging, and important problems remain open such as the nature of the ground state of a triangular lattice of antiferromagnetically coupled S=1/2 spins.

Trapped ions constitute an wonderful platform for the simulation of spin model Hamiltonians with long range interactions [POR04,ZHA17]. However, short-range interaction spin models, much more interesting to describe real materials, can not be handled this way. Here I propose a very different strategy: to use magnetic adatoms to carry out quantum simulations of 1D and 2D spin liquids. This is made possible due to several important discoveries in the last decade, some of them with my participation. First, the capability to fabricate spin arrays with up to 100 atoms on surfaces and to probe their spin excitations by inelastic electron tunneling spectroscopy (IETS) [HIR06,LOT12,SPI14, TOS16]. Second, the discovery that ability to these structures are accurately modelled with anisotropic Heisenberg models with short range interactions [HIR06, JFR09,LOT12, SPI14, TOS16]. Third, the invention of electron spin resonance driven by STM on individual atoms [BAU15]. This technique permits to probe low energy spin excitations with a spectral resolution 4 orders of magnitude improved, compared with IETS. It permits to use individual surface atoms as probe for the dipolar field of nearby atoms [CHO17] as well as the hyperfine splitting [WIL18b].

Here I propose a completely new strategy to carry out quantum simulations of the spin response function of spin liquids taking advantage of these recent experimental developments. Spin liquids are notorious for the lack of clear cut experimental smoking guns. Figure 4 describes the strategy that I will explore. The introduction of a magnetic impurity with large magnetic anisotropy structure of S=1/2 spins that forms as spin liquid induces a local magnetization, proportional to the non-local static spin-correlation function. This can be measured either with spin polarized STM (Fig. 4C) and much more precisely by probing the dipolar field doing an ESR-STM measurement on an external probe atom. This proposal provides a realistic modelling of all these phenomena, starting from the derivation of the spin model Hamiltonian from first principles, and solving them with DMRG.

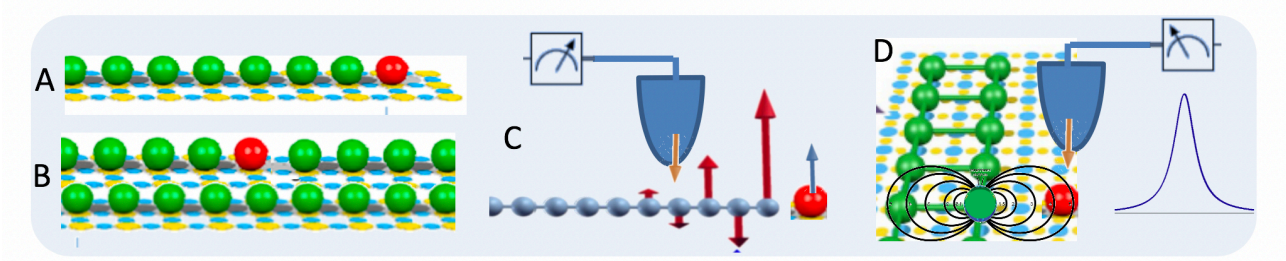

Figure *4.* Quantum simulation of spin liquids. A &. B *A chain and a ladder, made with S=1/2 atom (Ti on MgO), [YAN17], with a magnetic impurity, red ball, with very large magnetic anisotropy (for instance Co [RAU14]) in the edge(A) or in bulk(B),* ***that induces a local magnetization.*** **C** *SP-STM probing magnetization in A.* **D** *Nearby probe atom (red), such as Fe is used to probe spin noise and or magnetic field created by spin ladder. Figures adapted from [CHO17b] &[YAN17b]*

6. Time dependent spin model simulations: Optical exchange interactions

The two platforms considered so far target steady state quantum simulations of the equilibrium properties of the model Hamiltonians. The main reason is that a coherent manipulation of the relevant degrees of freedom is not possible on account of their short coherence time due to the proximity of an electron gas (see my review on magnetic adatoms [DEL17]). Here I look for an alternative strategy for spins localized in a wide semiconducting gap (>1.5 eV). It is based on the so called optical RKKY interaction between distant spins in semiconductors [PIE02,JFR04] that is induced by sub-gap laser radiation. The interaction is mediated by

virtual excitons that are present in the ground state of the semiconductor dressed with photons. The interaction is switched on and off with the laser field and does not require dissipative absorption processes.

Optical RKKY (ORKKY) would provide a very valuable resource to manipulate localized spins in semiconductors. The spins could come from nuclei, impurities or confined states. Indirect experimental evidence of ORKKY interaction has been reported for an ensemble of InGaAs quantum dots[SPA11], with a small strength, J= 1 μeV. This is too small if we want to use ORKKY for Analog Quantum simulations. Therefore, here I propose to explore ORKKY intereactions in the recently discovered two dimensional transition metal dichalcogenides (TMD) semiconductors, such as MoS_2.

TMD look very promising to explore ORKKY for several reasons. First, the two energy scales that enhance ORKKY, Rabi coupling [LIU15] and excitonic binding energy [WAN18], are much larger in TMD than in conventional GaAs and CdTe materials. Second, unwanted two-photon absorption is mitigated in atomically thin semiconductors. Third, surface functionalization of the 2D crystals could couple $N@C_{60}$ complexes with record spin coherence times [MOR07] (see figure 1C of this proposal).

I will carry out realistic calculations of the ORKKY interactions for a variety of TMD and local spins, starting from DFT calculations of the electronic structure[KOS13] of the host+impurity system, that yields a Kondo coupling between local spins and the carriers, the determination of the exciton wave functions, their photon dressing, and the tracing of the dressed excitons out of the Hamiltonian to obtain the spin-spin coupling.

7. Work plan and methods

This proposal has a unique grand goal: to pave the way to build analog quantum-simulation solutions to the quantum many-body problem. For that matter, the proposal defines, from the theoretical point of view, the roadmap to carry out analog quantum simulations using 3 different physical platforms. The work plan, detailed in B2, addresses the following goals: 1) the verification that the proposed platforms simulate the target model Hamiltonians, 2) the modelling of experimental probes that are feasible with state of the art and how they convey information of the simulated system, and 3) the validation of the simulated results.

The workplan requires a variety of methods I have used over the years, such as DFT based calculations of the electronic structure [JFR05,KOS13, FER15b, CAR18b ,SOR18], post-processing techniques to obtain tight-binding descriptions [KOS14,FER15a, FER15b,LAD16, LAD17, SOR18], exact diagonalization of models [JFR06, JFR09, DEL13, FER15a, FER15b], large scale quantum transport calculations [MUÑ09, LAD13], STM transport and IETS [JFR09, DEL13, KLE18], STM-ESR modelling [LAD17b,WIL18b], open quantum system decoherence calculations [DEL17], optical response calculations [JFR06, BES12], and optical RKKY calculations [JFR04,QUIN06] . I will also use some recent additions to my toolbox, such as **machine learning** [CAR18] and Density Matrix Renormalization Group [BAN17]. In addition, I will use some very novel techniques, such as **digital quantum simulations on real quantum computers**, that we are starting to explore in my group [GAU18].

8. Epilogue: Excellence, Impact and Relevance

This project has the potential to trigger an amazing revolution: the fabrication of efficient quantum simulators for the key model Hamiltonians that describe quantum matter. My background of successful collaborations with key players in the experimental fabrication of artificial lattices [SPI14,KAL16, YAN17,WIL18b] and 2D material devices [KLE18], together with my track record of relevant theory papers in the topics and methods of the proposed research [JFR04,JFR07, JFR09, KOS13], maximize the chances of success. In addition, at the time of writing I am already collaborating with the last author of the key paper for Objective 1 [GON16] in the modelling of his recent unpublished results in hydrogenated graphene.

QUASAL will define a realistic roadmap to fabricate 3 different quantum simulation platforms, relating the outcome of feasible experiments with the properties of model Hamiltonians. This roadmap will certainly focus the ongoing experimental efforts in the areas of surfaces spins and 2D materials towards a goal of undisputed importance: the ultimate solution of the quantum many body problem.

Success in the fabrication of efficient quantum simulation platforms would have far reaching consequences. We would not only solve problems that have challenged our community for decades, opening new venues and showing perhaps the road towards room temperature superconductivity. The implications of quantum simulations go beyond that, as they blur the frontier between experiment and theory, providing a radically new way of exploring the secrets of Nature.

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