Q@TN - Quantum Science and Technology in Trento

APPLICATION FORM

for PhD or postdoctoral fellowship

1. **Project title:** **Quantum simulator for Open Quantum Systems (QOQS)**
2. **Key words:** Out-of-equilibrium dynamics, ultra-cold gases, open systems
3. **Type of position requested:** Ph.D. student
4. **Duration of the position:** 3 years
5. **Estimated cost of the position**: 1 Ph.D. position: 68000€
6. **Managing Partner:** Department of Physics (UNITN)
7. **Proponents** : (full CV's attached to this submission)

- **Pietro Faccioli** (Associate Professor, Università degli Studi di Trento)

  a) E. Schneider, S. a Beccara, F. Mascherpa, and P. Faccioli. Quantum propagation of Electronic Excitations in Macromolecules: A Computationally Efficient Multiscale Approach. *Phys. Rev. B* **94**, 014306 (2016)

  b) J.-P. Blaizot, D. De Boni, P. Faccioli, and G. Garberoglio. Heavy quark bound states in a quark-gluon plasma: dissociation and recombination. Nucl. Phys. A 946, 49 (2016)

  c) E. Schneider and P. Faccioli. Long-Distance Quantum Transport Dynamics in Macromolecules. *Phys. Rev. B* **89**, 134305 (2014)

  d) E. Schneider, S. a Beccara and P. Faccioli. Dissipative Quantum Transport in Macromolecules: An Effective Field Theory Approach. *Phys. Rev. B* **88**, 085428 (2013)

  e) S. a Beccara, P. Faccioli, and G. Garberoglio. Quantum diffusive dynamics of macro-molecular transitions. *J. Chem. Phys.* **135**, 034103 (2011)

  Recently funded projects:

  i. Grandi Progetti di Ateneo 2014-2017 (role co-PI)

  ii. Serpin dynamics and function (Alpha-1 Fundation, USA) – participant

- **Giovanni Garberoglio** (Researcher, ECT*-FBK)

a) J.-P. Blaizot, D. De Boni, P. Faccioli, and G. Garberoglio. Heavy quark bound states in a quark-gluon plasma: dissociation and recombination. *Nucl. Phys. A* **946**, 49 (2016)

b) G. Garberoglio, S. Taioli, and S. Simonucci. The BEC–BCS crossover in ultracold Fermi gases beyond the contact-potential approximation. *Eur. Phys. J. D* **67**, 129 (2013)

c) G. Garberoglio and A. H. Harvey. Path-integral calculation of the third virial coefficient of quantum gases at low temperatures. *J. Chem. Phys.* **134**, 134106 (2011)

d) S. Simonucci, G. Garberoglio, and S. Taioli. Finite-range effects in dilute Fermi gases at unitarity. *Phys. Rev. A* **84**, 043639 (2011)

e) G. Garberoglio. Quantum states of rigid linear rotors confined in a slit pore: quantum sieving of hydrogen isotopes and extreme one dimensional confinement. *Eur. Phys. J. D* **51**, 185 (2009)

Recently funded projects:

i. Manager of the *Supercalcolo* initiative between FBK and Istituto Nazionale di Fisica Nucleare (INFN, Italian National Institute of Nuclear Physics). Development and application of numerical techniques in high-performance computing (total budget: 100000€)

ii. Manager and PI of several contracts with the National Institute of Standards and Technology (USA) for the high-accuracy calculation of virial coefficients of atomic and molecular quantum gases (total budget: 57000$)

- **Stefano Giorgini** (Associate Professor, Università degli Studi di Trento)

a) L. Parisi and S. Giorgini. Quantum Monte Carlo study of the Bose-polaron problem in a one-dimensional gas with contact interactions. *Phys. Rev. A* **95**, 023619 (2017)

b) L.A. Peña Ardila and S. Giorgini. Bose polaron problem: effect of mass imbalance on binding energy. *Phys. Rev. A* **94**, 063640 (2016)

c) L. A. Peña Ardila and S. Giorgini. Impurity in a Bose-Einstein condensate: study of the attractive and repulsive branch using quantum Monte Carlo methods. *Phys. Rev. A* **92**, 033612 (2015)

d) N. Matveeva and S. Giorgini. Impurity problem in a bilayer system of dipoles. *Phys. Rev. Lett.* **111**, 220405 (2013)

e) S. Pilati, G. Bertaina, S. Giorgini, and M. Troyer. Itinerant ferromagnetism of a repulsive atomic Fermi gas: a quantum Monte Carlo study. *Phys. Rev. Lett.* **105**, 030405 (2010)

Participation to the following projects:

i. "EuroQUAM-FerMix" project (European Science Foundation EUROCORES Program)

ii. ERC Advanced Grant "QGBE - Quantum Gases Beyond Equilibrium"

- **Alessio Recati** (Researcher, CNR-INO)

a) F. Scazza, G. Valtolina, P. Massignan, A. Recati, A. Amico, A. Burchianti, C. Fort, M. Inguscio, M. Zaccanti, G. Roati. Repulsive Fermi polarons in a resonant mixture of ultracold ^{6}Li atoms. *Phys. Rev. Lett.* **118**, 083602 (2017)

b) G. Valtolina, F. Scazza, A. Amico, A. Burchianti, A. Recati, T. Enss, M. Inguscio, M. Zaccanti, G. Roati. Exploring the ferromagnetic behaviour of a repulsive Fermi gas through spin dynamics. *Nature Physics* **13**, 704 (2017)

c) M. Klawunn, A. Recati. Polar molecules in bilayers with high population imbalance. Phys. Rev. A 88, 013633 (2013)

d) A. Recati, M. Klawunn. The Fermi-polaron in two dimensions: Importance of the two-body bound state. *Phys. Rev. A* **84**, 033607 (2011)

e) R. Combescot, A. Recati, C. Lobo, F. Chevy. Normal state of highly polarized Fermi gases: simple many-body approaches. *Phys. Rev. Lett.* **98**, 180402 (2007)

Participation to the following projects:

i. "EuroQUAM-FerMix" project (European Science Foundation EUROCORES Program)

ii. ERC Advanced Grant "QGBE - Quantum Gases Beyond Equilibrium"

Pietro Faccioli and Alessio Recati will be the formal supervisors of the Ph.D. student.

8. **The project is relevant for**:

- WP1, areas of action: Fundamental quantum physics; Quantum many-body physics; Quantum optics.

- WP4, area of action: Quantum Simulation for solid state and condensed matter.

9. **Description of the project:** (see below)

10. **Interdisciplinary aspects :** Cold atom Physics, quantum biology, nanotechnology

This project brings together scientists with different backgrounds but complementary skills, who have individually worked on different aspects of the physics of open quantum systems. SG and AR have a considerable expertise in many-body theory for ultra-cold gases and gave very important contributions to the development of the concept of Fermi- and Bose-polaron in this field [Lobo06]. PF has developed a framework based the path-integral formulation of quantum mechanics that enables a rigorous description of open systems in several interesting regimes. GG has been involved in the development of numerical implementation of this formalism, both in the case of a classical or quantum probe in an electrical plasma. The same path-integral formalism has been used to describe the dynamics of large classical objects (proteins) in their natural bath of water molecules, the dynamics of excitons in large molecules [Fac16], and the quantum dynamics of a pair of heavy quarks in an electrical plasma [DeB17], thus showing a great flexibility and potential for interdisciplinary applications.

The Ph.D. student will certainly strengthen the collaboration between the cold-atoms, the quantum biology, and the computational communities in Trento. Although the focus of this project is on the polaron problem, the student will operate in a multidisciplinary environment and will contribute to the development of theoretical and computational tools applicable to a wide range of problems, including – but not limited to – quantum biology and high-energy physics.

11. **Relevance of the project for quantum science and technology**

A deeper understanding of the polaron problem will certainly contribute to a better interpretation of experimental data on open quantum systems in several regimes, many of which are at the limit of validity of the traditional approaches.
Apart from the specific object of this research, we envision this project to be relevant also for other work packages. In particular, since the coupling of a quantum sensor with the system to be measured generally involves unwanted interactions with a larger environment, we expect that many of our findings will benefit the design and optimisation of activities related to the WP5 (Future sensors and metrology), thus fostering further collaborations with the corresponding activities in the local and national environment.

12. **Possible referees:**

i. Frederic Chevy. École Normale Supérieure, Paris, France.
   email: `frederic.chevy@lkb.ens.fr`

ii. Ines De Vega. LMU, Munich, Germany
   email: `ines.vega@physik.uni-muenchen.de`

iii. Matteo Zaccanti. LENS, Florence, Italy
   email: `zaccanti@lens.unifi.it`

iv. Tilmann Enss. Heidelberg University, Germany
   email: `enss@thphys.uni-heidelberg.de`

v. David Coker. Boston University, United States of America
   email: `coker@bu.edu`

vi. Benedetta Mennucci. Pisa University, Italy.
   email: `benedetta.mennucci@unipi.it`

Description of the project

Ubiquitous in quantum physics is the study of the *impurity problem,* a.k.a. the *polaron problem*, i.e., the investigation of the properties of a few particles or degrees of freedom immersed in a complex environment. This is one of the most relevant instances of *open quantum systems* (OQS), whose study encompass all the field of physics, both at the fundamental and — even more importantly — at a technological level. In the last 10 years, the interest in investigating the properties of decoherence and dissipation in OQS's has been boosted by the research in the fields of quantum information, quantum biology and quantum transport in nano-structures [DeVega17].

The impurity problem plays a key role in a number of different physical systems which are being investigated within the research institutes of Trento area. A list of examples includes ultra-cold atoms in fermionic, as well as bosonic baths, dipolar molecules in dipolar quantum fluids and crystals, excitons propagating in photosynthetic and biomimetic macromolecular complexes and heavy quarks diffusing in a super-hot quark-gluon plasma.

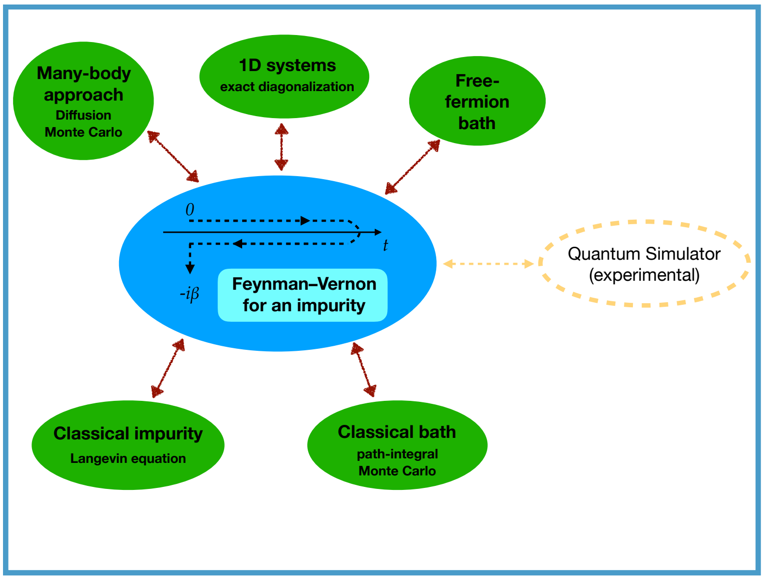
The theoretical modelling of these systems represents a formidable challenge both analytically and numerically, because of the huge number of degrees of freedom involved and because much of the interest is in investigating out-of-equilibrium properties. To cope with these challenges approximations and novel computational methods have been developed, tailored to the physical properties of the specific open quantum system under investigation. For example, in the study of fast quantum energy transfer processes in macromolecules, the atomic nuclei can be considered as a thermalised heat-bath of classical particles [Fac16]. In addition, for short times or weak exciton-vibron coupling the reduced density matrix for the excitonic degrees of freedom can be obtained analytically, using a diagrammatic perturbation theory [Fac13]. In contrast, in the study of super-hot strongly interacting matters, the heavy quarks generated in an ultra-relativistic heavy ion collision may be described as classical and non-relativistic probes, diffusing in a thermal bath of quantum and relativistic light quarks and massless gluons [Gar10, Gar16]. In this case, the perturbative expansion is justified only in the high-temperature regime. The advantage of describing some degrees classically, while retaining a full quantum description for others has also driven several technical development in the theoretical setup. In particular, many of these studies are performed within a framework in which some degrees of freedom are described in quantum field theory and other in first quantisation, and the reduced density matrix for the polaron is calculated using the Feynman-Vernon path integral representation.

In the context of cold gases the polaron problem has become an area of study by itself. Novel techniques, e.g., time-dependent variational approaches, or short time dynamics, have been introduced to describe the outcomes of the relative large number of experimental results around the world. The static properties for both bosonic and fermionic baths have been described in details, by means of variational, diagrammatic and Monte-Carlo techniques. Scientists at the Trento University and of the CNR in Trento gave major contributions in the very idea of polaron or impurity in cold gases [Rec03, Lobo06, Gio08] as well as in developing new many body techniques many of the techniques used in the field [Com08, Rec11, Gio15]

Clearly, each of the research lines on OQS's developed in Trento would highly benefit from a systematic assessment of the accuracy of the approximations listed above. From a more general and cross-disciplinary standpoint, identifying the asymptotic regimes in which these approximations can be rigorously justified and assessing their validity in a range of physical parameters would significantly advance the understanding of the quantum behavior of open systems.

In this context, Feynman quantum simulators made of cold atoms provide test systems with ideal properties. Indeed, fundamental parameters such as the system's effective dimensionality, the strength of the interaction, or the temperature of the bath can be well controlled, enabling different asymptotic regimes to be experimentally realized. Furthermore, in these systems is even possible to follow the dynamics of the impurity in real-time.

The purpose of this proposal is to test the different OQS's techniques and approximations by applying them to specific cold-atom quantum simulators, which can be experimentally realised and characterised in an external partnering laboratory at the European Laboratory for Non-Linear Science, at Sesto Fiorentino (PI Dr. Giacomo Roati). We attach to this submission a supporting letter



The PhD candidate will learn various theoretical and numerical methods. He/she will learn diagrammatic and path integral approaches to perturbation theories as well as numerical techniques for solving multidimensional differential equations and Monte-Carlo approaches. In order to accomplish such rather ambitious task he/she will take advantage from the direct guidance of the researchers who are expert in or have even directly developed the different analytical and numerical methods. The different techniques will be used to tackle different regimes of few impurities immersed in a bath. Such a learning stage will bring the candidate at the front line of the contemporary theoretical research in OQS's. At the same time the obtained results could be compared with some of the most recent experiments in the cold gases field, in order to both validate the theory approximated theories and hopefully to get new insights in the still unexplained experimental outcomes. The candidate will have the possibility to join various meeting to discuss her/his results with our external experimental partner in Florence. The meetings will be also devoted to plan and design open cold atom systems to reproduce the different asymptotic regimes where the underlying theory approximation apply. In the spirit of using cold gases as a quantum simulator for more complex and less flexible physical systems.

Finally, in the last stage of the project, the candidate will investigate how different approximations fail in the regions of parameters space where asymptotic approximations are no longer holding.

Resources: The project will be carried at the Department of Physics and the PhD candidate will have access to the facilities of the department, as well as those at FBK. In particular, concerning the computational part the candidate will have access to the FBK cluster "KORE", with 1250+ cores and 8.5 TB RAM and 30 NVIDIA GPUs.

Estimated Costs:

1 PhD position	68 K€

Travels, workshop organization, visitors and publications	20 k€ (on INO-CNR funds)
Total	88 k€

Deliverables: A Ph.D. thesis and several publications on international high-profile and peer-reviewed journals. We will organise an international conference during the year 2020, corresponding to the middle of the duration of the Ph.D. position. We will submit a proposal in this direction to ECT*, which has the institutional commitment of promoting workshops and collaboration meetings in theoretical nuclear physics and related areas, including many-body quantum physics, Bose–Einstein condensation, and computational physics, all of which are a significant part of this proposal.

References:

[DeB17] "Fate of in-medium heavy quarks via a Lindblad equation". J. High Energ. Phys. (2017) 2017: 64

[DeVega17] "Dynamics of non-Markovian open quantum systems", Inés de Vega and Daniel Alonso. Rev. Mod. Phys. 89, 015001 (2017)

[Fac13] "Dissipative Quantum Transport in Macromolecules: An Effective Field Theory Approach", E. Schneider, S. a Beccara and P. Faccioli, Phys. Rev. B 88, 085428 (2013).

[Fac16] "Quantum propagation of Electronic Excitations in Macromolecules: A Computationally Efficient Multiscale Approach", E. Schneider, S. a Beccara, F. Mascherpa,, P. Faccioli, Phys. Rev. B 94, 014306 (2016)

[Gar10] "A Path Integral for Heavy Quarks in a Hot Plasma", A.Beraudo, J.P. Blaizot, P.Faccioli, G. Garberoglio, Nucl. Phys. A 846, 104 (2010).

[Gar16] "Heavy Quark Bound States in the Quark-Gluon Plasma: Dissociation and Recombination", J.-P. Blaizot, D. De Boni, P. Faccioli, and G. Garberoglio Nucl. Phys. A 946, 49 (2016).

[Gio08] "Phase Separation in a Polarized Fermi Gas at Zero Temperature", S. Pilati and S. Giorgini, Phys. Rev. Lett. 100, 030401 (2008).

[Gio15] "Impurity in a Bose-Einstein condensate: Study of the attractive and repulsive branch using quantum Monte Carlo methods", L. A. Peña Ardila and S. Giorgini, Phys. Rev. A 92, 033612 (2015).

[Lobo06] "Normal State of a Polarized Fermi Gas at Unitarity", C. Lobo, A. Recati, S. Giorgini, and S. Stringari, Phys. Rev. Lett. 97, 200403 (2006).

[Rec05] "Atomic Quantum Dots Coupled to a Reservoir of a Superfluid Bose-Einstein Condensate", A. Recati, P. O. Fedichev, W. Zwerger, J. von Delft, and P. Zoller, Phys. Rev. Lett. 94, 040404 (2005).

[Rec08] "Fermi polaron in two dimensions: Importance of the two-body bound state", R. Combescot, A. Recati, C. Lobo, F.Chevy, Phys. Rev. Lett. 84, 033607 (2011).

[Rec11] "Fermi polaron in two dimensions: Importance of the two-body bound state", M. Klawunn and A. Recati, Phys. Rev. A 84, 033607 (2011).