

**ERC Starting Grant
Research proposal (Part B2)**

Section 2: The Project proposal

(references for sections a and b can be found at the end of section b)

Introduction

This research project is motivated by the potentially numerous applications of a technique that has been recently developed by the PI and collaborators, that goes under the name of *quantum cavity method*, and is capable to describe a broad class of strongly interacting disordered systems. Typical examples are systems of disordered fermions or bosons, and quantum spin glasses. Given the generality of the setting, we expect the method to have many potential applications to concrete physical problems arising in different fields: indeed, we have in mind applications to fields as diverse as quantum computing and condensed matter. Moreover, via the standard mapping between quantum Hamiltonians and stochastic processes, the results of this project will also be relevant for the stochastic dynamics of classical systems, with applications in chemistry, biology and information theory; this constitutes an interesting perspective for future developments.

For the sake of concreteness, we will initially focus on some specific problems that have recently emerged in the first two fields mentioned above (namely, quantum computing and condensed matter), on which we believe that progress can be made in the short term using the quantum cavity method. These problems include:

- (i) **Adiabatic quantum computing:** Some quantum algorithms exploit quantum fluctuations to find the ground state of classical spin-glass like disordered Hamiltonians. The Hamiltonian describing the quantum computer is therefore that of a quantum spin glass. It is commonly believed that these algorithms will run into problems if the quantum computer undergoes a phase transition during the optimization process. Hence, the study of the phase diagram of quantum spin glasses is essential to assess the performances of these quantum optimization algorithms.
- (ii) **Localization in presence of interactions:** The question whether an interacting system can display Anderson localization is strongly debated since the original Anderson paper of 1958. Exact solutions of interacting models are very important in this context and may shed light on the problem and confirm or disprove recent results based on perturbation theory. These results should also be relevant in connection with experiments on disordered cold atomic systems, in the experimental quest for a Bose glass phase.
- (iii) **Superfluidity and superconductivity in disordered systems:** Many aspects of superfluidity in a disordered environment are still poorly understood: for instance, in disordered solid phases, such as the recently proposed superglass phase. These exotic phases are observed in Helium 4 confined in porous media or by producing “dirty” crystals by fast quenches from the liquid phase. Moreover, they could be observed in cold atoms assemblies in presence of disordered external potentials.

What are the reasons why these problems are so hard? Why do we believe that a common treatment of them is possible? The answer to these questions is that all these problems share the following common ingredients, that complicate a lot their theoretical description:

- **disorder/frustration:** frustration means that each degree of freedom of the system is subject to competing interactions, that give it contradictory indications. For instance, for a given Ising spin, some interactions could favor the “up” state while others could favor the “down” state. In this situation, many *locally stable* and *inhomogeneous* states appear, and the description of the system becomes much more complicated than that of homogeneous systems characterized by only a limited number of possible states.
- **strong interactions:** the presence of strong interactions makes the problem difficult because perturbation theory, which is one of the main tools to study interacting systems, becomes completely ineffective. Non-perturbative phenomena become important and one has to find new methods to understand them.
- **quantum fluctuations:** the quantum nature of the problem constitutes an additional complication, because quantum strongly interacting problems are technically more difficult to handle than their classical counterparts already in absence of disorder and strong interactions. Moreover, new physical phenomena (such as tunnelling between different locally stable states, or interference effects leading to localization) appear, that are completely absent in the classical limit.

The interplay between all these effects makes the theoretical description of these systems a very difficult task. Most of the standard methods of theoretical physics suffer from severe drawbacks when applied to these problems. For instance, mean field theory assumes the existence of an “effective” background field produced by the whole system and hence fails to capture the spatial fluctuations due to disorder; numerical methods such as Quantum Monte Carlo are severely limited by ergodicity problems and slow dynamics, hence they only allow to study small systems; the renormalization group is very difficult to formulate in presence of frustration, already for classical

systems. On the other hand, the problem is very general and common to different fields: making progress towards its general solution will be very beneficial for several concrete problems, leading also to cross-fertilization between different domains.

Why do we believe, with reasonable confidence, that some progress on this difficult problem can be achieved in the near future?

In a nutshell, the answer to this question is that a method, the quantum version of the so-called “cavity method” (also known as the “Bethe approximation” in condensed matter and “Belief Propagation” in information theory), specifically designed to tackle these problems, has very recently become available. The method is based on a mean field treatment of these systems and allows for a full analytical solution of the problem within this approximation. It allows to handle the presence of several locally stable states in a compact way, at the same time keeping track of local fluctuations which are essential in the study of these problems. Moreover, the method includes, in special limits, some recently developed theories such as Dynamical Mean Field Theory (DMFT). The method is still in the earliest stage of its development, but it already allowed to the PI and his collaborators to obtain important results and predictions on the phase diagram of these systems [CTZ09,JKSZ10,FSZ10a]. The main aim of this project is its further development, and its application to the physical problems described above.

We expect to obtain several new results, the most important being:

- **full computation of the phase diagram of quantum optimization problems**, such as random satisfiability, exact cover, and the coloring of random graphs. Instances of these problems are standard benchmarks for quantum computation, and these results will give important indications on the performances of quantum adiabatic algorithms in solving them;
- **exactly solvable models displaying a Bose glass phase**; this result will be important to give indications on the nature of the superconductor-insulator transition in strongly disordered materials, elucidating the relation between the Mott (interaction-driven) and Anderson (disorder-driven) localization mechanisms and providing a good model to study Many-Body Localization effects. They will find applications in the physics of cold atoms and that of disordered superconducting electrons, since Cooper pairs can be treated as Bosons;
- **a complete theory of the superglass phase**; the existence of this phase has been recently proposed by mean of numerical simulations and analytical arguments. It might exist in Helium 4, but it is expected to be very difficult to observe in experiments. This study will allow to obtain information on what are the crucial features of the interaction potentials (attractive or repulsive? two-body, three-body, or more?) that give rise to this phase. This will help to identify the right system to observe this phase in experiments.

In the following, we will provide additional details on the background (section a), on the methodology and on the expected results (section b), and on the resources that are needed for the success of the project (section c).

a. State-of-the-art and objectives

In this paragraph we will discuss in details the theoretical background for the specific fields on which the project will initially focus. We will present the physical setting, explain what are the problems and challenges, and identify specific objectives to be solved during the project.

a1. Adiabatic quantum computing: a quantum algorithm for optimization

The theoretical research on quantum computing is motivated by the exciting perspective of computers that take intrinsically advantage of the laws of quantum mechanics. Besides the great effort of research towards the physical realization of these devices, a lot of activity has been devoted to the development of “softwares”, that is algorithms that could use the specific properties of quantum computers to achieve a faster velocity in performing computational tasks with respect to classical devices. Some of the quantum algorithms proposed up to now have been written with a specific task in mind (for instance factoring a large integer [S97]). A typical problem that is encountered in almost all branches of science is that of optimizing irregularly shaped cost functions: the Quantum Adiabatic Algorithm (QAA) [FGLLP01], also known as quantum annealing [KN98], is an adaptable proposition that is in principle able to tackle such problems in an universal way. Suppose one wishes to find the ground state of an Hamiltonian HP acting on N qubits of the quantum computer. To run the QAA one considers a simpler Hamiltonian HQ , such that the quantum computer can be easily initialized in the ground state of HQ . If one slowly interpolates the Hamiltonian $H(t)$ of the quantum computer from HQ (at time $t=0$) to HP (at a final time $t=T$), the adiabatic theorem ensures that, with high enough probability, the system will remain at all times in the ground state of the interpolating Hamiltonian. Hence, at the end of the evolution, it will be in the ground state of HP and the original problem will be solved. The crucial question is of course how slow the evolution should be, in the thermodynamic limit in which the number of qubits N goes to infinity. The total time T needed to ensure adiabaticity is expected to diverge for large N , and one would like in particular to distinguish between a polynomial and an exponential scaling of T with N , for large N .

Quite generally, the adiabaticity condition requires the rate of change of $H(t)$ to be smaller than the (squared) gap between the ground state and the first excited state of $H(t)$. Hence, the time needed to ensure adiabaticity will diverge in the thermodynamic limit whenever a quantum phase transition, at which the gap is expected to vanish [S99], is encountered during the interpolation between HQ and HP.

It is well established that the gap vanishes *at least polynomially* in N at a quantum second order critical point [S99] (except in some cases in presence of disorder, where it might exhibit a stronger dependence on N [F95]), while it vanishes *exponentially* in N at a first order phase transition [JKKM08]. Hence, establishing the presence of phase transitions and their nature is of extreme importance to assess the performances of the QAA on these problems.

The formal computational complexity theory [GJ79] classifies the difficulty of a problem according to a worst case criterion. It might however well be that “most” of the instances of a given problem are easy, even though a few atypical instances are very difficult. To give a precise content to this notion of typicality the research has turned to the study of random ensembles of instances, defining a probability distribution on the space of instances. The difficulty of these instances is usually controlled by a parameter c , that quantifies the amount of constraints put on the degrees of freedom of the problem, and which corresponds to the average connectivity of the underlying random graph. They provide a tunable benchmark of instances very useful for evaluating the typical performances of algorithms, and in fact the proposition of [FGLLP01] was made on such random instances. Rephrasing the open issue of above, we can say that a major goal of research should be the determination of the typical efficiency of the quantum adiabatic algorithm in the thermodynamic limit, as a function of the control parameter c . A classical example is the famous *graph coloring problem* (q -COL): one is given a graph of N vertices, and a set of q possible colors (for $q=3$, one could choose blue, red and green). The problem is the following: *does it exist an assignment of colors to each vertex, such that no pair of vertices connected by a link of the graph have the same color?* Suppose we look to the ensemble of *all* possible graphs of average connectivity c . It might well be that there is a “worst” graph for which finding the answer to this question is very difficult, although for most graphs the answer can be found very easily. Depending on the application one has in mind, studying the worst or the typical case might be more relevant. In this project we will focus on typical cases. For instance, in the q -COL problem, one may pick graphs at random among all graphs that have average connectivity c and study the typical properties with respect to this measure over graphs. This is known as *Random q -COL*.

Combinatorial optimization problems (the Hamiltonian HP one is typically interested in) can be represented as classical spin models [MPV87]. For instance, the q -COL problem can be reformulated as follows: we represent the color of each node by a Potts spin assuming values from 1 to q . The Hamiltonian HP is a classical Potts antiferromagnet: if two spins connected by an edge have different values, the energy is zero, while if the two spins have the same value, one pays a fixed energy price. For a given graph, the q -COL amounts to the following question: *does the Potts antiferromagnet on this graph have a zero-energy ground state?* If the answer is yes, then the graph is colorable. Random q -COL amounts to find the ground state energy of a Potts antiferromagnet defined on a random graph of average connectivity c . In more general cases the Hamiltonian HP will contain quenched disorder and hence will be a *spin glass*. Therefore, determining the generic phase diagram of Quantum Spin Glasses is essential to investigate the performances of the QAA in solving these problems. This problem has intensively been investigated in the past decade, and early results generated considerable excitement by reporting polynomial scaling of the minimum gap for sizes up to $N \sim 100$ [FGLLP01, YKS08]. The problem is that all these studies rely on the study of very small systems and/or on perturbation theory. Moreover, particular choices of random ensembles of instances have been made in [FGLLP01, YKS08], by selecting instances that have a single ground state. This is conceptually dangerous since generically random optimization problems have many degenerate solutions, and their difficulty could be underestimated by this restriction. Indeed, it has been recently established [MZ97, MPZ02, KMRTSZ07] that the exponential degeneracy of the ground state in these problems can lead to a very complex structure, characterized by a series of non-standard phase transitions upon varying the parameter c . What is the quantum analog of these phase transition? Are they characterized by a vanishing gap, and if yes, what is the scaling of the gap for large N ? These questions remain at present completely open.

To summarize in a few words the above discussion:

- The QAA is a versatile algorithm that can tackle a variety of optimization problems of great practical importance. It amounts to slowly change the Hamiltonian $H(t)$ of the quantum computer to follow adiabatically its ground state.
- An important benchmark for the QAA are random optimization problems like Random q -COL. The quantum Hamiltonian associated to these problem is a Quantum Spin Glass. It is characterized by strong frustration, coming from the different conflicting constraints that have to be solved (otherwise the problem would be easy).
- Assessing the performances of the QAA is related to finding the scaling of the minimum gap of the Hamiltonian $H(t)$ in the thermodynamic limit. Since the gap is expected to vanish at quantum phase transitions, and the scaling of the gap is connected to the nature of the transition, the first task is to fully characterize the phase diagram of Quantum Spin Glasses. The second task is to understand the behavior of the gap at the quantum analogs of the exotic phase transitions that are encountered in classical limit of these problems.

The two tasks defined above constitute two main objectives of this project. Solving them will be a considerable advance in the field of quantum information: indeed, as already stated, assessing the performances of "quantum softwares" is of extreme practical importance to motivate research oriented towards the realization of quantum computers. Additionally, a more complete understanding of the structure of quantum optimization problems might result in the design of more efficient quantum algorithms: this is indeed what happened in the classical case, where a new very efficient algorithm, known as *Survey Propagation (SP)*, has been proposed by physicists [MPZ02] based on the understanding of the structure of the classical problem that has been recently achieved [MZ97, MPZ02, KMRTSZ07].

a2. Quantum fluctuations and disorder in condensed matter systems: many-body localization, superfluidity and superconductivity in disordered environments

Quantum particles moving in a disordered environment exhibit a plethora of non-trivial phenomena. The competition between disorder and quantum fluctuations has been the subject of vast literature since the milestone papers [A58, FWGF89], with a renewed interest following the exciting frontiers opened by the experimental research with cold-atoms [FFI08, BG08]. One of the most striking features resulting from the presence of a disordered external potential is the appearance of localized states [A58], that is driven by interference effects in presence of disorder. Localization happens both for Fermions and Bosons, but in the latter case one has to introduce repulsive interactions to prevent condensation of particles in the lowest energy state. This results in the existence of an insulating phase called "Bose glass" [FWGF89], which is observed in Helium 4 absorbed in porous media and more recently in cold atomic systems [FFI08, BG08]. This localization mechanism, driving the formation of an insulating phase, is very different from the interaction-driven localization, originally proposed by Mott [M68], in which the formation of an insulator is related to strong hopping suppression due to the repulsion between particles. Indeed, the Bose glass is characterized by a finite compressibility and gapless density excitations in striking contrast with the Mott insulating phase [FWGF89]. Yet, it is believed that these two mechanisms coexist in many realistic materials close to the superfluid-insulator transition [W09], giving rise to interesting phenomena, in a region of parameters where interactions and disorder are so strong that perturbation theory completely breaks down and the theoretical description of the system becomes extremely challenging. To further complicate the picture, latest research stimulated by the possible discovery of a supersolid phase of Helium [KC04] has led to the theoretical foresight of a "superglass" phase [BPS06, BCZ08], corroborated by recent experimental evidence [S09, HPGYBD09], where a metastable amorphous solid features both condensation and superfluidity, in absence of any random external potential. The apparent irreconcilability between the current picture of insulating "Bose glasses" and the emergence of this novel phase of matter calls for a better understanding of the physics of Bose-Einstein condensation in strongly disordered quantum glasses. Achieving this better understanding for the technically simpler case of Bosons will have also an important impact on Fermions: paradigmatic example are the electron glass [DLR82, BOP93] and the superconductor-to-insulator transition driven by disorder in thin films [GM98, HP90], which has been related in some cases to a Bose glass transition of Cooper pairs [FWGF89, M09].

In addition (and in connection) to the above problems, a very basic question in quantum statistical mechanics is whether a system made of an infinite number of interacting degrees of freedom can act as a heat bath for a given subsystem of itself. The first suggestion that certain infinite systems may fail to do so was already contained in the original Anderson paper about localization [A58]. This long-standing problem can be rephrased as follows: is it possible that transport coefficients of an infinite interacting quantum system are strictly vanishing at finite temperature? A lot of activity in this field has been generated by a recent paper [BAA06], claiming to have demonstrated that this is indeed possible. It was predicted in [BAA06] that a system of interacting electrons in presence of strong enough disorder will undergo a finite-temperature phase transition between a completely insulating low-temperature phase, characterized by a strictly vanishing conductivity, and a standard high-temperature phase where conductivity is possible through activated hopping between localized levels. This result is based on perturbation theory and one can be worried that non-perturbative terms may wash out the effect. The problem is very difficult because the transition is not associated to any obvious order parameter; one has to resort to exact diagonalization of small systems, and using standard finite-size-scaling techniques seems not very useful to establish the existence of the transition [OH07, BR10, PH10]. Recently, it has been suggested that this phenomenon might have important phenomenological implications for the physics of Bose glasses discussed above [M09]. Exact (non-perturbative) solutions of interacting models are very important in this context and may shed light on the problem and confirm or disprove the general picture proposed in [BAA06, M09].

From a theoretical point of view, all these systems are usually described by variations of the Hubbard Model, whose Hamiltonian is made by the sum of a hopping term, a local on-site repulsion, and possibly other short range interactions. Both Fermionic and Bosonic versions of the Hubbard model have been considered in the literature. Unfortunately, exact solutions of these models could be obtained only in one dimension [G04] and in special cases. In higher dimensions, information about the behavior of the model came mostly from perturbative expansions around special limits (zero hopping, zero interaction, low density), and more recently from exact diagonalization

[PH10] and Quantum Monte Carlo (QMC) numerical simulations [BS96, PST98, GPPST09]. There were attempts to resum classes of diagrams of a given perturbative expansion, but these resummations are difficult to control.

A standard way to tackle difficult interacting problems is mean field theory. In the case of Bosons, an earlier attempt to formulate a mean field theory was performed in [FWGF89] where a fully connected lattice was considered (particles could hop from each site to any other). However in this limit both spatial and quantum fluctuations are frozen and, for instance, the Bose glass phase disappears. A recent important development was the formulation of a consistent mean-field theory of the Fermionic Hubbard model, that goes under the name of Dynamical Mean Field Theory (DMFT) [GKKR96]. DMFT proved to be a good approximation for finite dimensional models and provided important insight into the Mott transition and the emergence of superconductivity. Its generalization to take into account disorder [DK97] was capable to describe both the Mott and Anderson transitions in the respective limits of zero disorder and zero interaction giving important indications on the regime where the two mechanisms are simultaneously at work. One of the virtues of DMFT is that it is exact in a controlled and still non-trivial limit, namely when the number of neighboring sites where a particle can hop is very large (for instance in very large spatial dimension). In principle well-defined expansions around this limit are possible. Bosonic DMFT (B-DMFT) has only recently been formulated in a consistent way [BV08]. This is due to a technical difficulty in performing the large connectivity limit, related to the possible presence of a Bose-Einstein condensate. Despite its many successes, the main drawback of DMFT is that in the limit in which it is exact (infinite dimension) localization effects disappear. Indeed the extended DMFT of [DK97] can only be thought as an approximation of a finite dimensional system, and at variance to standard DMFT it does not become exact in any well controlled limit. At the same time, the subtleties associated with the physics of localization in presence of strong interactions, disorder and frustration strongly call for exact solutions, as discussed above. This is required to avoid making predictions that might turn out to be only artefacts of the approximations made.

This is precisely what we intend to achieve in this project through the development of the quantum cavity method for particle systems. In fact, the cavity method has the virtue of being a good approximation of finite dimensional systems, at the same time being *exact* on a class of lattices that locally look like trees and go under the name of Bethe lattices (indeed the cavity method is a refinement of the so-called Bethe approximation). In Bethe lattices, each site has a finite connectivity, or in other words the number of neighbors where a particle can hop is kept finite: this allows to retain spatial fluctuations, and indeed it was shown that the Anderson delocalization transition can happen on such lattices [ATA73]. This is a striking result and shows that the Bethe lattice is indeed the simplest candidate to discuss the physics of localization in presence of strong interactions. Remarkably, DMFT has also been formulated on Bethe lattices in the limit of infinite connectivity [GKKR96]. Another advantage of the Bethe lattice is that it is amenable to numerical studies using Quantum Monte Carlo or Density-Matrix Renormalization Group (DMRG) and Matrix-Product States [SDV06, NFGSS08, PP08]. Recently, a new type of glassy phase of electrons (Valence Bond Glass phase), due to the interplay of quantum fluctuations and magnetic frustration, has been predicted on the Bethe lattice [BT08]. Finally, a one-dimensional lattice can be viewed as a special tree (with connectivity two), therefore Bethe lattices allow to interpolate in a simple way (by changing the connectivity) between one-dimensional and infinite-dimensional models.

To summarize in a few words the above discussion:

- The study of quantum particles moving in a disordered environment, either due to an external potential (e.g. impurities) or self-induced by frustration, is obviously important in almost all aspects of condensed matter systems. Concrete examples, that will be addressed in this project, are Bose glasses (recently realized in cold atoms), superglasses (that might have been recently observed in Helium 4), electron glasses, and superconductor-to-insulator transitions driven by disorder in thin films.
- Additionally, the problem of localization in presence of interactions is a very fundamental one in quantum statistical mechanics, being related to the ability of a quantum system to act as a bath for its subsystems.
- In both problems, elusive and subtle effects play important roles, and one is in a regime of parameters where interaction and disorder are strong, and perturbation theory might not be reliable. Hence, exact solutions are of key importance to obtain a clear picture of the problem.
- Bethe lattices provide exactly solvable models: this has been successfully exploited in the non-interacting case, showing that Anderson localization is possible. But up to now only an approximate treatment has been possible in the interacting case, by means of DMFT.

Our task in this part of the project will be to exploit the quantum cavity method to obtain the exact solution of interacting models on the Bethe lattice, fully including frustration effects, glassy physics, and localization effects. We strongly believe that this will have an important impact in this field, since this study will be able to shed light on fundamental issues such as the physics of the localization transition in presence of interactions, the difference between Bose glasses and superglasses, and the interplay of Mott and Anderson localization mechanisms close to the metal-insulator transition.

b. Methodology

Having identified the main objectives of the project and explained the physical context, we now turn to the discussion of the methodology we will use to make progress on them and eventually come to a solution.

b1. Methodological background:

All the examples above belong to a wider class of problems where the interplay between *quantum fluctuations*, *strong interactions* and *disorder/frustration* plays a key role. Indeed, the models that have been used to investigate these problems are strikingly similar. Typically, the quantum Hamiltonian is the sum of a “classical” part that contains strong interactions and disorder, and a term inducing the quantum fluctuations (hopping for particles, or a transverse field for spins). The “classical” part of the Hamiltonian can typically be reduced to a classically frustrated system, such as a Random Field Ising Model or a spin glass. Therefore, one can expect that these problems can be tackled by properly translating to the quantum world our experience in the study of classically frustrated systems. *This is the main methodological objective of this project.*

Why do we believe, with reasonable confidence, that some progress on all these apparently different problems can be achieved in the near future? In a nutshell, the answer to this question is that a method, the quantum version of the so-called *cavity method*, was very recently developed by a Princeton group [LSS08] and a French based group involving the PI [KRSZ08]. The method is still in its earliest stage: many technical problems have yet to be solved, and we believe that technical progress will lead to very interesting results when the method will be applied to the different problems listed above. We will now explain why.

Our main aim in this project will be that of developing a method to compute *quantitatively*, within reasonable approximation, the phase diagram of a wide class of quantum strongly interacting disordered Hamiltonian. This is extremely difficult, mainly because due to the strong interactions, perturbation theory (that is the standard way of tackling difficult quantum problems) breaks down. Note that we will not focus on the critical regime close to a phase transition, hence sophisticated techniques such as the Renormalization Group are of little help in this case. Apart from special cases (mainly one dimensionals) where one can obtain exact solutions [G04], two main strategies to tackle these problems have become standard nowadays: on the analytical side, one often resorts to mean-field like theories; on the numerical side, one makes use of Quantum Monte Carlo simulation schemes. However, both methods, despite many successes, suffer from severe drawbacks when applied to disordered strongly interacting systems.

Numerical simulations are difficult for several reasons. First of all, strongly disordered and glassy systems are characterized (almost by definition) by ergodicity problems. The standard strategy to compute thermodynamic properties of quantum systems is to exploit the Feynman path-integral formulation of quantum mechanics and map the quantum problem into a classical one, where the original quantum variables are replaced by their classical *imaginary time trajectories*. A proper sampling of the probability distribution of these paths is already technically difficult in standard cases. For disordered and glassy systems, the equilibration time becomes so large that in practice one is limited to very small systems [GBH94]. A second difficulty is that one has to average over many independent samples (or equivalently consider very large samples) in order to properly take into account rare realizations of the disorder, that are often relevant in determining the physical behavior of the system in the thermodynamic limit close to the quantum critical point [GPPST09,W09]. The behavior of small systems is sometimes misleading, as the scaling with system size can change dramatically for larger systems. Striking examples of this are the Bose glass phase [GPPST09,W09] and Griffiths phases in quantum disordered magnets. Hence, although numerical simulations can give very precious indications, analytical methods that are capable of taking directly the thermodynamic limit and the average over the disorder are very much needed.

The other traditional tool is the mean field approach, in which one assumes that the behavior of the system can be captured by a “representative” degree of freedom subject to a “mean external field” which is averaged over the whole system. The latter is determined self-consistently by assuming that the representative degree of freedom describes the environment of its neighbors. However, disordered systems are strongly heterogeneous, and each degree of freedom feels a very different local field coming from its local environment. The interplay of heterogeneity and quantum fluctuations is at the basis of the interesting phenomena observed in such systems. Another important ingredient that has to be taken into account by the theory is that frustration often induces the existence of a very large number of *metastable states* (i.e. local minima of a suitable free energy functional), each described by a different set of local fields. Hence, solving these problems requires the development of a method capable of taking into account the strong fluctuations of the local fields, while at the same time being analytically solvable in the thermodynamic limit, and being able of performing the correct average over the disorder.

b2. The cavity method

In the classical case, a consistent mean field description of frustrated systems has been achieved by the so-called *cavity method* [MP01]. This method is designed to tackle exactly a physical situation in which local fields display strong fluctuations from site to site, and from one metastable state to the other. Its more elaborate versions allow to deal with glassy phases that arise in frustrated spin models and which manifest themselves by the proliferation of the number of metastable states. This method has been very successfully applied in the context of random combinatorial optimization, thanks to the analogy between these problems and finite connectivity mean-field spin-glasses. There are two different and complementary ways in which this method can be described, that we now discuss in some details.

i) First of all, the cavity method provides the exact solution of models defined on Bethe lattices. Before illustrating this point in detail, let us stress that in this context, the word “exact solution” means that the method allows to reduce the computation of the partition function of a system made of many interacting degrees of freedom to the solution of *a single equation*. Clearly this equation will be complicated and in most cases one will have to solve it numerically, but the important point is that the thermodynamic limit is taken from the beginning, avoiding the need of complicated finite-size scaling procedures to detect, for instance, phase transitions. Given this remark, we now turn to the definition of a Bethe lattice. A Bethe lattice has often been defined in the literature as a rooted tree. However, in the case of frustrated spin models (spin-glasses) some care has to be paid in the definition of a Bethe lattice because of the importance of the boundary conditions for models defined on trees. Indeed, the “surface” (the number of leaves) of a rooted tree of N sites scales as its “bulk” in the thermodynamic limit of large N , which creates several technical problems: for instance, extensive quantities like the free energy are dominated by boundary effects. The most satisfying definition of a Bethe lattice corresponds to a random regular graph [MP01], namely a graph chosen uniformly at random in the set of graphs in which each vertex has the same number of neighbors. In other words, one considers the set of all possible graphs of N sites, such that each site is connected to exactly c other sites, and gives the same probability to each graph in this set. It can be shown that typical graphs in this ensemble locally look like trees, since the size of their loops diverges as $\log(N)$. Yet, all sites are statistically equivalent, hence there is no boundary: the graph is statistically “translationally invariant”. In the following we shall use “Bethe lattice” and “random graph” as synonymous. Note that with this definition in terms of random graphs it is straightforward to incorporate, if necessary, local quenched fluctuations of the environment of a spin like a fluctuating local connectivity.

The cavity method exploits the locally tree-like structure of random graphs to provide the exact solution of the model. This is possible because classical models on trees are very simple to solve. Indeed trees have a natural recursive definition, that allows to solve independently the models on sub-trees, and glue the solutions together to construct the one of a larger tree. In random graphs the structure of interactions is a tree only locally; the cavity method is a way to incorporate in a self-consistent way the effect of the long loops, that act as a boundary condition on the tree portions of the graphs. This effect can be of different type depending on the amount of constraints the interactions put on the degrees of freedom. When these are weak enough the correlations between variables decay rapidly with the distance, the system is almost insensitive to the presence of the loops and the local recursions derived exactly on the tree remain exact in the random graph for N going to infinity; in this case the cavity method is equivalent to the Bethe approximation or the Belief Propagation method. Increasing the intensity of interactions (for instance lowering the temperature) this property might not hold anymore, if one encounters a phase transition. The description of the transition is relatively easy if one enters a phase with a finite number of pure states that can be easily characterized (for instance the two states of positive and negative magnetization of a ferromagnet at low temperature); one can always break explicitly the symmetry between the pure states (for instance with a small magnetic field) and effectively recover the simple situation described above. The problem becomes however much more difficult in mean-field disordered systems, where the number of pure states can grow exponentially in the size of the system, with no obvious way to select one of them. This is where the cavity method is most useful and provides a convenient way to deal with this proliferation of pure states (mean-field glassiness).

ii) A different perspective on the cavity method is to consider it as a “refined” mean-field like approximation (the so-called *Bethe approximation*) of models defined, for instance, on a square or cubic lattice. The Bethe approximation is the second in a hierarchy of mean field approximations. To illustrate this let us consider a given variable of the system. In standard mean field theory one neglects not only the correlations between neighbors of a given variable, but also the feedback that a given variable has on its neighbors. In the Bethe approximation the latter assumption is removed: one still treats the neighbors as independent in absence of the reference variable (as they would be on a tree), but at the same time one takes fully into account the correlations among the neighbors induced by the reference variable. Indeed, the Bethe approximation is quantitatively much more accurate than standard mean field: we recently demonstrated this fact in the case of the Bosonic Hubbard model [STZ09].

In summary, the cavity method can be seen as the exact solution of Bethe lattice models or as a “refined” mean-field like approximation (the Bethe approximation) of models defined on a square or cubic lattice. Moreover, this method has several important advantages:

- 1) It takes into account local spatial fluctuations of the environment, and the existence of many different states; it allows to take the thermodynamic limit and in this limit it allows to compute probability distributions of local observables with respect to disorder;
- 2) It can be formulated via a variational principle: in other words there is a suitable free energy functional whose minimization yields the cavity equations; this allows a direct access to the free energy of the system, and makes easy to devise variational approximations to the true solution.
- 3) It allows to define a distance between two spins as the number of interactions on a shortest path between them, leading to a consistent definition of a correlation length.

b3. The method that will be used in this project: the quantum cavity method

From a technical point of view the goal of this project is to develop a full generalization of the cavity method to quantum models, suitable to be applied to the diverse problems outlined above. Indeed, in the quantum case the cavity method allows to study phenomena that are intrinsically related to the notion of distance, the most striking of them being Anderson localization [ATA73], that can be studied on a Bethe lattice while it disappears in the standard mean field limit of infinite connectivity. The main technical difficulties in this program come from the fact that quantum models on trees are already much more difficult than their classical counterparts. The global configuration of the system in the classical case can be easily decomposed into the configurations of the various branches around a node taken as the root, and the total classical energy as the sum of contributions arising from each branch. Turning instead to a quantum system, the global configuration is described by a vector in the total Hilbert space (the wavefunction). This, in general, cannot be written as the tensor product of vectors of the Hilbert space spanned by the spins of the various branches. In other words the configurations of the subtrees are *entangled*.

To overcome this problem, it has been proposed in [LSS08] to use the same path integral formulation that is used in Quantum Monte Carlo. Thanks to this formulation the variables of the quantum model are replaced by their classical imaginary time trajectories; in [LSS08] a discretization of time (Suzuki-Trotter) was used. The PI and his collaborators improved over this preliminary investigation by showing how to perform the continuum imaginary-time limit, and they applied the method to solve exactly the quantum Ising ferromagnet in a transverse field on a random regular lattice [KRSZ08]. In a subsequent paper we showed how to generalize the method to Bosonic systems [STZ09]. In this way, the cavity method allows to reduce the solution of the model to the problem of finding the fixed point of a functional equation for the local effective action for imaginary time paths. In two subsequent works appeared on Phys.Rev.Lett. [CTZ09, JKSZ10], we included in the quantum cavity method a crucial ingredient that has been developed in the classical case (known in jargon as replica symmetry breaking effect), that is needed to treat the most interesting situations, where many metastable glassy states are present. Including these effects does not pose any particular conceptual challenge, but increases considerably the computational cost of the numerical solution of the cavity equations. These results constitute the basic starting point of this project, whose objective is the further development of the method and its application to other interesting physical problems.

The cavity equations are complicated recurrence equations for the local effective action, and one has to find their fixed point. At variance with DMFT equations, in which only the leading Gaussian term is kept, in the cavity method one *explicitly takes into account all many-points local correlations in time*, therefore having access to the full local effective action. However, the equations are difficult to handle. The strategy introduced in [KRSZ08] consists in constructing a sample of spin trajectories from the local effective action and finding statistically a fixed point by iterating the cavity equation on this sample. This method has been shown to work well for spin and Bosonic models where the matrix elements of the Hamiltonian in the Suzuki-Trotter representation are all positive and the effective action is then a probability distribution. However, this method is limited because it cannot access directly the zero-temperature limit, and it does not work for cases (such as fermions or the real-time dynamics of bosons) where a sign problem arises. It is desirable to develop alternative strategies that could address, possibly in an approximate way, these more complicated cases.

It is important to stress at this point the relation between our formulation of the quantum cavity method and other attempts to go beyond the simplest mean-field theory for disordered quantum systems. As already discussed, the quantum cavity method is *exact* on random graphs (Bethe lattices). It turns out that it contains, as special limits, many different methods that have been very recently developed to investigate these problems. These all correspond to large connectivity limits, in particular:

- 1) The stochastic mean-field theory of [BH09] and the closely related method of [IM10] both correspond to the leading order in a large connectivity expansion of the cavity method, for bosons and spins respectively.
- 2) A certain class of extensions of the Fermionic DMFT [DK97] correspond to the leading order in large connectivity of the cavity method for fermions.
- 3) The recently formulated Bosonic DMFT [BV08] and the original formulation of [LSS08] take into account the next-to-leading order in the same expansion for bosons and spins, respectively.

In some cases we will make use of these methods in this project. This will allow to simplify the computations in order to extract the physics more easily when a complete solution of the cavity equations will be too demanding, at the price of loosing part of the information on the local quantum dynamics, which is treated exactly in the cavity method. However, we will always check the results against the solution of the full cavity equations, whenever possible. The fact that so many cavity-like approximations have been recently derived testify the vitality of the method in the present moment.

b4. Specific goals of the project in the short term

Technical problems to be solved:

Based on the above considerations, here follows a list of technical issues that we will have to solve in order to achieve some of the goals of this project:

- a) Find reliable and efficient approximation schemes to solve the quantum cavity equations, possibly of a variational nature, and/or based on large connectivity expansions as in DMFT. These methods should work down to zero temperature. More concretely, we believe that the static approximations developed in [IM10] could be very helpful to give indications on the qualitative behavior of complicated models.
- b) Extend the method to Fermions. In this case, a path-integral formulations in the basis of occupation numbers (such as the one used in [STZ09]) gives rise to negative path weights that generate sign problems in the stochastic procedure that we used in [KRSZ08, STZ09], that becomes ineffective. A possible way out of the problem is based on a different path integral formulation in term of Fermionic (Grassmanian) coherent states. In this formulation the signs are automatically taken into account by the anticommuting nature of Grassman variables. The problem becomes that of parametrizing the local effective action, that is a functional of Grassman paths. We plan to do this at first by discretizing time; in this case the action is easily parametrized, however the number of parameters scales exponentially in the number of time slices. We will try to find ways to optimize the computation for large number of slices.
- c) Optimize the efficiency of our code for the solution of replica symmetry breaking quantum cavity equations. Indeed, the preliminary investigations of [CTZ09, JKSZ10] required a considerable computational effort, at the limit of our current capacities. Improving over these results crucially requires a more efficient code and improved computational power. Hence, the task is to optimize as much as possible the algorithms that are used in the computation (which will require some conceptual work to improve the sampling techniques we are currently using), and make heavy use of parallelism to speed up the execution of the code. Fortunately, the algorithm we proposed in [KRSZ08, JKSZ10] can be very naturally and efficiently parallelized.

However, it is important to stress that many applications that will be discussed in the rest of this section can already be tackled with the existing machinery of the quantum cavity method. We will now explain in more details, for each domain of application of the method, what are the technical challenges and the expected results; we will also provide a specific list of mid-term objectives for the project.

(i) Adiabatic quantum computing:

As it has been discussed in the background section above (section a, part (i)), assessing the performances of the Quantum Adiabatic Algorithm is related to finding the scaling of the gap of a spin glass Hamiltonian in the thermodynamic limit. Since the gap is expected to vanish at quantum phase transitions, and the scaling of the gap is connected to the nature of the transition, the first task is to fully characterize the phase diagram of Quantum Spin Glasses. The second task is to understand the behavior of the gap at the exotic phase transitions that are encountered in these problems. We already performed a preliminary investigation [JKSZ10] of the simplest optimization problem, namely the random XORSAT problem in a transverse field. XORSAT is a system of linear equations on Boolean variables, each of the form $x+y+z=b$, where the sum is modulo 2 and $b=0,1$. In random XORSAT one picks at random the variables entering in each clause among N variables, and chooses for each equation the term b at random in $0,1$. The structure of the solution space of this problem in the classical case has been rigorously established [CDMM03, MRZ03], and we made use of these results and of the quantum cavity method to understand how this structure is modified when adding quantum fluctuations to the problem. We showed that this problem displays a first order quantum phase transition as a function of the quantum fluctuations intensity. This transition is accompanied by an exponentially small gap in the thermodynamic limit, which makes the QAA

ineffective for this problem [JKSZ10]. In this project we plan to continue this line of research by extending this study to other problems in order to assess the universal features of their phase diagram. More concretely, our program is the following:

(i.1) We will investigate more complex optimization problems, such as the coloring of random graphs described above, and random satisfiability (random k-SAT). These problems have a much richer structure already at the classical level, that has been described only recently by mean of the classical cavity method [KMRTSZ07]. We expect their quantum extensions to display a rich phase diagram characterized by different quantum phase transitions of exotic nature, related to the glassiness of the classical problem, or in other words to the large degeneracy of its ground states. We will compute the phase diagram of these problem in the thermodynamic limit and taking the average over the disorder.

(i.2) The exponentially large (in the number of variables) degeneracy of the ground and excited states of these problems should have an important impact on the minimum gap and on the performances of the QAA. In such a situation the relevant gap probably involves the excited states that are not continuously transformed to the degenerate classical ground states. Preliminary results pointing in this direction have been very recently obtained [AKR09, FGGM09, FSZ10b]. To address this problem, one should study the spectrum of the Hamiltonian on given instances of the problem of fixed size, and then study the scaling as a function of system size and the distribution over the disorder. We plan to investigate this question by exact diagonalization on toy models involving a small number of variables, yet which present such a degeneracy of levels. Later we will extend this study to the more realistic problems described above, being guided by the knowledge of the system's properties in the thermodynamic limit obtained previously.

(ii) Localization in presence of interactions (*Many-body localization*):

The application of the cavity method to the problem of many-body localization (explained in the second part of the background section above, section a part (ii)) has been recently initiated in [IM10]. However, in this paper some not well-controlled approximations within the cavity method have been made. Since the problem is highly controversial, this first study is an important guideline, but needs to be improved and confirmed by an exact solution of the cavity equations in order to exclude that the results are artefacts of the approximation. Technically, the difficulty comes from the fact that the transition is of a dynamical nature and therefore requires to obtain information on the real time dynamics of a given model. We will achieve this by the following strategy:

(ii.1) We will initially focus on the simplest candidate to show such a transition, namely, a one dimensional Heisenberg spin chain in a random transverse field. We will solve the model by the cavity method (recall that the method is exact in one dimension) and compare the solution in the thermodynamic limit with exact diagonalization results for small instances [PH10, BR10]. This should allow to identify the correct order parameter for the transition.

(ii.2) Then we will turn to the same model defined on a Bethe lattice of fixed connectivity. In this case very interesting predictions have been made in [IM10] by means of an approximate solution: in particular it has been shown that the problem displays a low-temperature glassy phase where the magnetic susceptibility is dominated by rare fluctuations. We will check these predictions accurately by means of the exact cavity computation.

(ii.3) Finally, we will investigate the disordered Bose-Hubbard model [FWGF89], for which a huge amount of QMC data [GPPST09] are available, and that is most relevant for experiments [FFI08, BG08]. If successful, this study will be important in several aspects: first of all, we will provide an exactly solvable model that shows a Bose glass phase; second, we will compute precise numerical values for the transition predicted in [IM10], that should be helpful to look for this phase in experiments; third, we will check the recent phenomenological proposal of [M09] that uses concepts of many-body localization in order to explain the superconductor-to-insulator transition in thin disordered films.

(iii) Superfluidity and superconductivity in disordered systems:

We will initially focus on Bosonic systems. They are technically easier, and their investigation is very timely since cold-atoms experiments recently provided access to exotic phases of disordered bosons [FFI08, BG08]. In a preliminary investigation, we already confirmed, by mean of the cavity method, an earlier suggestion [BPS06, BCZ08] that geometrical frustration alone can induce a “superglass” phase of bosons in which the system supports at the same time glassy ordering and superfluidity [CTZ09]. We then investigated quantum extensions of lattice glass models, that are simply obtained by adding an hopping term to the Hamiltonian studied in [BM02], and established their phase diagram by the cavity method [FSZ10a]. We found a very interesting phase diagram. At low enough temperature the glass transition line is re-entrant as a function of the strength of quantum fluctuations, meaning that a glass can be formed upon increasing quantum fluctuations at fixed density. Similar results have been obtained by the group of D.Reichman at Columbia University using a different method [MMBMRR10]. In addition, we showed that the glass transition becomes a first order superfluid-insulating glass transition at zero temperature, accompanied by a phase coexistence between the two phases. In other words, in a given region of the

phase diagram one might have a coexistence, in the same sample, of glassy and superfluid regions. This result will contribute to the current, highly controversial, theoretical and experimental debate about the very nature of superfluidity in solid Helium. We also expect this phase diagram to be quite similar to the one of random SAT and coloring, hence the study of these problems (task i.1 above) will allow to check the degree of “universality” of phase diagrams of quantum glassy systems.

We plan to continue this new line of research by studying the existence of superglass phases in more realistic models and try to understand which are the relevant features of the interactions that determine their existence. In particular:

(iii.1) We will make use of the expertise we acquired on simpler models to design a finite-dimensional lattice model with realistic interactions, that could be realized in cold atomic gases, and that could exhibit a superglass phase. We will simulate the model via Quantum Monte Carlo in order to provide a detailed phase diagram that should serve as a guide for experiments designed to find this new phase of matter.

(iii.2) We will apply these concepts to off-lattice models, in order to clarify the relation between lattice superglassy phases and the recently proposed supersolid phase of bulk Helium [KC04] through accurate quantitative computations. We will then extend the computation to other systems, for instance particles interacting via dipolar interactions, in which glassy phases might be more easily detected in experiments. We will do this by three complementary techniques:

(iii.2a) We will improve over the variational method of [BCZ08]; the latter employed the simplest variational wavefunctions for Helium (of the Jastrow form), while much better wavefunctions are known, such as the Shadow wavefunctions. We will repeat the calculation of [BCZ08] for these wavefunctions, which should allow to obtain an accurate zero temperature glassy phase diagram for Helium.

(iii.2b) We will adapt the replica method that has been developed in the past decade to obtain a quantitative theory of classical glasses [MP99, PZ10] to the quantum case. It is worth to note that the PI has acquired a solid experience on this subject, and he recently wrote a review of the method for Rev.Mod.Phys. [PZ10]. The method is based on a combination of the replica approach and of standard liquid theory, and is extremely successful in the classical case to locate the glass transition temperature and to compute correlation functions of glasses. The exact solution of quantum lattice glass models that we recently obtained [FSZ10a] will serve as a guide to extend it to the quantum case.

(iii.2c) We will perform Path Integral quantum simulations to confirm numerically our findings. Since these simulations are extremely demanding, having obtained an analytical estimate of the transition lines will be extremely useful to find the good range of parameters that we will investigate numerically.

For Fermions the problem is technically much more difficult, yet we think that progress can be made in this direction, as discussed above. In addition to the problem of formulating the cavity method for Fermions, we will explore other complementary research directions:

(iii.3) In the large connectivity limit, the cavity method reduces to the disordered extension of DMFT introduced by [DK97]. We plan to extend this method by including replica symmetry breaking effects, that are needed to describe frustrated glassy situations characterized by many amorphous metastable states. A natural application of this method is the study of the electron glass [BOP93, DLR82].

(iii.4) Another natural application of the method is the description of cold Fermionic gases in a disordered environment [FFI08]. In this case the temperatures that are currently achieved are not much lower than the Fermi temperature. Hence, a description using a discretization of imaginary time with a moderate number of slices might be enough to obtain reasonable results on the experimental scales.

b5. Perspectives for a longer term research

(iv) Stochastic dynamics of disordered systems

After most of the research outlined above will be completed, we will turn to the application of the method to classical dynamics. Indeed, it is well known that the master equation describing the Markovian stochastic dynamics of a classical system can be mapped onto a quantum Hamiltonian. Hence, similar methods can be used to tackle both problems. Dynamical problems involving a large number of interacting entities in presence of disorder are encountered in a wide class of applications: examples are the analysis of stochastic algorithms in computer science and of gene regulatory networks in biology. It is difficult to exhaust here all the potential applications of the method in this context. At present we plan to focus initially on the following two studies, but we expect that many other interesting application will emerge during the development of the project.

(iv.1) Classical optimization problems are often solved by mean of stochastic algorithms that perform a random walk in the space of configurations according to some local update rule. It can be proven in many cases that for random instances, a given algorithm will be effective, in the thermodynamic limit, up to a given *algorithmic threshold* in the ratio of clauses to variables (which is a simple measure of the “difficulty” of a problem). Above the threshold the algorithm fails with very high probability. The analytical computation of algorithmic thresholds has

been performed only in very simple cases; by mean of the dynamic cavity method we will be able to compute it for a much wider class of algorithms, and hopefully to obtain insight into the structural reasons that make these algorithms fail.

(iv.2) In many applications to chemistry and biology one is interested in the computation of *transition rates* between different stable states of a network. For large systems, it is tempting to identify these states as metastable states. Hence, one would like to compute transition rates between different metastable states of the network. We expect this to be possible for sparse random networks by mean of the dynamic cavity method, combined with standard sampling methods like the one proposed in [DBCC98]. An interesting example of an application is to gene regulatory networks; these are characterized by a complicated stochastic dynamics, in which the expression of each gene is regulated by a number of other genes. Describing this dynamics is challenging but very important to understand the functioning of these networks.

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c. Resources (incl. project costs)

The structure of the project requires working in parallel on several distinct (although related) research directions, and to perform a lot of computational work. For this reason, a team of at least three persons working at full time on the project, coordinated by the PI, is necessary. The team will be composed by the PI and by two post-doc fellows per year at the beginning, or one post-doc and one PhD student for the three last years of the project. We will also provide support to two young researchers that will work part time on the project, to help the team members for some specific tasks, and allocate some money for visiting students from other EU countries.

Personnel: the core of the team

The PI has a permanent CNRS position which gives him total freedom to work on his research projects. He has no obligation of any kind (apart from performing excellent scientific work) with respect to its institute. He has no teaching duties. Hence, he will be committed at 80% to the project without the need of any direct funding (leaving a 20% free time for implication in other projects, students supervision, etc.). The total actual cost of PI salary is 6167 euros/month (74000 euros/year); 80% of the salary (59200 euros/year) should be funded directly by the project budget.

Every year of the project, two persons will work under the direct supervision of the PI; they are central figures of the project. They will bring experience on specific topics (such as Quantum Monte Carlo and other numerical methods) and perform both analytic computations and numerical simulations. Post-docs will be hired on “junior” positions (less than 2 years of research experience from PhD, approximate cost 4083 euros/month or 49000 euros/year) and on “senior” positions (more than 2 years of research experience from PhD, approximate cost 4520 euros/month or 54250 euros/year). We will open at first two “two-years junior positions”; on the third year we will open one “three-years senior position” (see table below), and at the same time a PhD student will join the project. The student will be supported for three years (33000 euros/year).

We expect this arrangement to keep a good equilibrium in the team, since in the initial (more critical) phase of the project the two “junior” post-docs will work in parallel and in direct collaboration with the PI, while in the last three years when the project will be more advanced, the “senior” post-doc will help the PI in supervising the student, whose activity will focus on some specific tasks, among the objectives of the project, that will emerge at that time as promising and yet not too risky.

Personnel: collaborators and visiting students

The PI has a long standing collaboration with Italian colleagues from Rome and Trieste in joint supervision of PhD students. This co-supervising activity will be pursued by allocating some money (10000 euros for the first two years, and 5000 euros for the other years) to support PhD students from other European countries wishing to spend long or short periods of research in France working on this project under the PI supervision, in collaboration with their supervisors in their home country. These students will provide additional manpower to perform specific tasks, and at the same time these collaborations will contribute to circulation of ideas related to the project among the EU.

Finally, the team will be completed by two associates. In the French system, young researchers are often appointed as Assistant Professors (Maitre de Conference, MdC). These are permanent teaching/research positions that however require an important teaching charge (192 hours per year). Universities allow them to reduce their teaching duties if the corresponding part of their salary is paid by a third institution. Hence 20000 euros/year will be used to discharge two young MdC from a part of their teaching, so that they will be able to participate part-time to the research activity related to the project. These MdC will be selected, each year, based on scientific excellence and on the complementarity of their skills with the rest of the team. They will bring specific expertise to the project, acting as “consultants” on specific topics.

Other direct costs:

The calculations needed for the success of the project require a substantial computational power. In order to take full advantage of the parallelization of the code, a cluster of at least 320 cores is needed. The cluster will be bought at the beginning of the project and will serve during the full duration (5 years) of the project. To speed up communication between the cores and optimize the parallelization, we will use 32-core blades, the current standard of technology. We estimated the price of one such blade by asking for a quote to the Dell official seller in France. The best option is to use Dell PowerEdge R815 blades, each equipped with 4 processors AMD Opteron 6136, 8 cores each, 2.4GHz, 4M Cache. The price for one such blade is 7068 euros including taxes. We will need at least 10 such blades, therefore we consider a total price of 70680 euros which we round to 75000 euros to take into account a possible increase of prices during the next year.

The success and dissemination of the project requires to keep important contacts with the leading groups in the field (many European groups, the MIT group of Prof. Farhi, the Princeton group of Prof. Sondhi, etc.). Therefore it will be necessary to allocate a substantial amount of money for travelling. While it is not obvious to estimate the money needed for travelling each year, we considered around 4000 Euros per year for the PI, 2000 euros for each Postdoc and the PhD student, and 1000 euros for each senior associate. This amounts to approximately 10000 euros per year. Some money (3000 Euros per year) will also be used to invite collaborators from other Institutions (indicated in 'Other').

Finally, the overheads are estimated as 20% of the total budget.

	Cost Category	Year 1	Year 2	Year 3	Year 4	Year 5	Total (Y1-5)
Direct Costs:	<i>Personnel:</i>						
	PI	59200	59200	59200	59200	59200	296000
	Senior Staff	20000	20000	20000	20000	20000	100000
	Post doc J1	49000	49000	0	0	0	98000
	Post doc J2	49000	49000	0	0	0	98000
	Post doc S1	0	0	54250	54250	54250	162750
	PhD Student	0	0	33000	33000	33000	99000
	Support for EU students	10000	10000	5000	5000	5000	35000
	Other	0	0	0	0	0	0
	Total Personnel:	187200	187200	171450	171450	171450	888750
	<i>Other Direct Costs:</i>						
	Equipment	75000	0	0	0	0	75000
	Consumables	0	0	0	0	0	0
	Travel	10000	10000	10000	10000	10000	50000
	Publications	0	0	0	0	0	0
	Other	3000	3000	3000	3000	3000	15000
	Total Other Direct Costs:	88000	13000	13000	13000	13000	140000
	Total Direct Costs:	275200	200200	184450	184450	184450	1028750
Indirect Costs (overheads):	Max 20% of Direct Costs	55040	40040	36890	36890	36890	205750
Subcontracting Costs:	(No overheads)						
Total Costs of project:	(by year and total)	330240	240240	221340	221340	221340	1234500
Requested Grant:	(by year and total)	330240	240240	221340	221340	221340	1234500

For the above cost table, please indicate the % of working time the PI dedicates to the project over the period of the grant:

80%

d. Ethical issues

ETHICS ISSUES TABLE

Research on Human Embryo/ Foetus		YES	Page
	Does the proposed research involve human Embryos?		
	Does the proposed research involve human Foetal Tissues/ Cells?		
	Does the proposed research involve human Embryonic Stem Cells (hESCs)?		
	Does the proposed research on human Embryonic Stem Cells involve cells in culture?		
	Does the proposed research on Human Embryonic Stem Cells involve the derivation of cells from Embryos?		
	I CONFIRM THAT NONE OF THE ABOVE ISSUES APPLY TO MY PROPOSAL	X	

Research on Humans		YES	Page
	Does the proposed research involve children?		
	Does the proposed research involve patients?		
	Does the proposed research involve persons not able to give consent?		
	Does the proposed research involve adult healthy volunteers?		
	Does the proposed research involve Human genetic material?		
	Does the proposed research involve Human biological samples?		
	Does the proposed research involve Human data collection?		
	I CONFIRM THAT NONE OF THE ABOVE ISSUES APPLY TO MY PROPOSAL	X	

Privacy		YES	Page
	Does the proposed research involve processing of genetic information or personal data (e.g. health, sexual lifestyle, ethnicity, political opinion, religious or philosophical conviction)?		
	Does the proposed research involve tracking the location or observation of people?		
	I CONFIRM THAT NONE OF THE ABOVE ISSUES APPLY TO MY PROPOSAL	X	

Research on Animals		YES	Page
	Does the proposed research involve research on animals?		
	Are those animals transgenic small laboratory animals?		
	Are those animals transgenic farm animals?		
	Are those animals non-human primates?		
	Are those animals cloned farm animals?		
	I CONFIRM THAT NONE OF THE ABOVE ISSUES APPLY TO MY PROPOSAL	X	

Research Involving non-EU Countries (ICPC Countries)		YES	Page
	Is the proposed research (or parts of it) going to take place in one or more of the ICPC Countries?		
	Is any material used in the research (e.g. personal data, animal and/or human tissue samples, genetic material, live animals, etc) :		
	a) Collected in any of the ICPC countries?		
	b) Exported to any other country (including ICPC and EU Member States)?		
	I CONFIRM THAT NONE OF THE ABOVE ISSUES APPLY TO MY PROPOSAL	X	

Dual Use		YES	Page
	Research having direct military use		
	Research having the potential for terrorist abuse		
	I CONFIRM THAT NONE OF THE ABOVE ISSUES APPLY TO MY PROPOSAL	X	