NKFI	Identifier:	151294	STARTING
	Assigned panel:	MATHINF, PHYSICS	
	Project to supplement:		
Type: STARTING Duration: 48 (2025-01-01 - 2028-12-31) Budget plan: 55 422 000 HUF	Specialties: permission is not necessary		

Title:	Quantum Generalizations of Markov Chain Monte Carlo Methods		
Keywords:	Metropolis, Glauber, Quantum		
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Specialty and related panel:

40%	Mathematics	Mathematics, Computing Sciences, Informatics
40%	Computing science	Mathematics, Computing Sciences, Informatics
20%	Physics	Physics

Evaluation panel proposed: Mathematics, Computing Sciences, Informatics (MATHINF)

Interdisciplinary evaluation requested: No

Brief summary of the research data expected to be produced during the course of the project, including their nature, quantity, handling of the occasional risks, and your plans for data management, long-term conservation and accessibility::
We do not plan to generate data beyond a few numerical values presented in the publications.

Are you going to use international research infrastructure in the project?:	No
Are you going to purchase (expand/upgrade) research infrastructure (instrument) within the project?:	No
Are you planning in-house development of instrument (equipment) within the project?:	No

Summary

Summary of the research and its aims for experts

Describe the major aims of the research for experts and evaluators of the proposal.

Describe here briefly the problem to be solved by the research, the starting hypothesis, and the questions addressed by the experiments. Describe the new perspectives opened by the results achieved, including the scientific basics of potential societal applications. Please describe the unique strengths of your proposal in comparison to your domestic and international competitors in the given field.

During my PhD at the University of Amsterdam I studied quantum algorithms under the supervision of Ronald de Wolf and Harry Buhrman, and my main objective was to find novel quantum approaches that provide fundamental quantum advantage over classical algorithms. A major achievement was the development of the Quantum Singular Vale Transformation (QSVT) framework that enables performing linear algebra operations on a quantum computer in a native way. I continued this research during my postdoc years at the California Institute of Technology where my mentors were John Preskill and Fernando Brandao. Not much after I arrived at Caltech, Fernando Brandao established the Amazon Web Services Center for Quantum Computing just across the campus, and asked me to join their team. I, however, decided to start a Marie Curie Fellowship at the Rényi Institute but kept working with Fernando and one of his PhD students, Chi-Fang Chen, in the framework of a sponsored research agreement. This collaboration led us to the discovery of novel quantum algorithms that we consider the faithful generalization of classical Markov Chain Monte Carlo (MCMC) methods. We recently found some subsequent variants, and the time is ripe to develop a deeper mathematical understanding of these algorithms, hopefully leading to practical quantum applications. I also plan to apply for an ERC Starting grant with a related topic.

MCMC methods, particularly the Metropolis algorithm and Glauber dynamics, are foundational techniques for simulating the behavior of large, complex systems that have become indispensable across various fields, including computational physics, biology, and finance. The power of MCMC methods is that they effectively work with an exponentially large stochastic matrix and simulate its effect by choosing appropriate probabilistic transitions among basis states without needing to explicitly apply matrix operations. Quantum generalizations of MCMC methods aim to leverage quantum superposition and entanglement to explore the state space more efficiently.

Previous attempts to generalize classical MCMC methods to quantum systems failed due to the inherent quantum uncertainty in learning properties of quantum states that hindered designing appropriate transitions or ``jumps'', breaking detailed balance and / or the efficiency of sampling, which are crucial for the success of these algorithms. However, we recently found a new breakthrough approach that incorporates quantum transitions in a coherent fashion while preserving the desirable properties of the classical methods. I plan to explore further generalizations, extensions and improvements over these constructions.

Understanding the mixing times, which measure the speed of convergence to the equilibrium distribution, is another critical step in obtaining efficient algorithms. A recent result by Rouzé et al.'24 shows that for high-enough temperature the process we described converges in polynomial time, which is the first known results in the general non-commuting case, and heavily relies on the detailed balanced properties of our construction. I plan to establish new comprehensive bounds and to understand the factors influencing the mixing times in different quantum systems. This could help understanding how to choose the jump or transition operators, and apply other system-specific fine-tuning of the general algorithms.

The successful development and understanding of quantum generalizations of MCMC methods could herald practical quantum algorithms for demonstrating a clear quantum advantage. By enabling simulations that are infeasible for classical computers, these algorithms could revolutionize various domains, from material science to financial modeling, offering unprecedented computational power. This research aims to advance the theoretical framework of quantum algorithms as well as to realize tangible benefits that underscore the transformative potential of quantum computing.

Summary and aims of the research for the public

Describe here the major aims of the research for an audience with average background information. This summary is especially important for NRDI Office in order to inform decision-makers, media, and others.

Markov Chain Monte Carlo (MCMC) methods, are foundational techniques for simulating the behavior of large, complex systems that have become indispensable across various fields, including computational physics, biology, and finance. The core of the technique is a simple iterative process exploring the state space of a system through local updates, allowing for the approximation of the equilibrium distribution efficiently. The power of MCMC methods is that they effectively work with an exponentially large stochastic matrix and simulate its effect probabilistically without needing to explicitly apply matrix operations by choosing appropriate probabilistic transitions among basis states.

In the quantum case the goal is to sample from a distribution over quantum states, and a quantum computer in principle can apply a similar strategy, designing appropriate transitions among quantum states -- which can be a superposition of exponentially many basis states. Quantum generalizations of MCMC methods aim to leverage quantum superposition and entanglement to explore the state space more efficiently.

The successful development and understanding of quantum generalizations of MCMC methods could herald practical quantum algorithms for demonstrating a clear quantum advantage. By enabling simulations that are infeasible for classical computers, these algorithms could revolutionize various domains, from material science to financial modeling, offering unprecedented computational power. This research not

only aims to advance the theoretical framework of quantum algorithms but also aspires to realize tangible benefits that underscore the transformative potential of quantum computing.

1 Excellence and background

During my PhD at the University of Amsterdam I studied quantum algorithms under the supervision of Ronald de Wolf and Harry Buhrman, and my main objective was to find novel quantum approaches that provide fundamental quantum advantage over classical algorithms. A major achievement was the development of the Quantum Singular Vale Transformation (QSVT) [GSLW19] framework that enables performing linear algebra operations on a quantum computer in a native way. QSVT turned out to be an extremely valuable tool for processing quantum information in an efficient way with low quantum space and time overheads. I demonstrated this through improved algorithms related to statistical problems such as distribution testing and entropy estimation [GL20] as well as for implementing Petz recovery maps and pretty good measurements [GLM$^+$20].

I continued this research during my postdoc years at the California Institute of Technology where my mentors were John Preskill and Fernando Brandao. Not much after I arrived at Caltech, Fernando Brandao established the Amazon Web Services Center for Quantum Computing just across the campus, and asked me to join their team. I, however, decided to start a Marie Curie Fellowship at the Rényi Institute but kept working with Fernando and one of his PhD students, Chi-Fang Chen, in the framework of a sponsored research agreement. This collaboration led us to the discovery of novel quantum algorithms that we consider the faithful generalization of classical Markov Chain Monte Carlo (MCMC) methods. We recently found some subsequent variants, and the time is ripe to develop a deeper mathematical understanding of these algorithms, hopefully leading to practical quantum applications. I also plan to apply for an ERC Starting grant with a related topic.

The topic of this research proposal is the study of dissipative algorithms that are quantum analogues of the classical Metropolis algorithm and Glauber dynamics, also known as quantum Gibbs sampling. This is related to the constructive quantum Lovász Local Lemma [GS17], which is a quantum generalization of the classical constructive Lovász Local Lemma [EL75, MT10]. While the classical variant aims to sample a solution of certain "sparse" constraint satisfaction problems, the quantum algorithm tackles the analogous problem of preparing the ground state of certain frustration-free "sparsely constrained" Hamiltonians. Similarly to the case of quantum Metropolis sampling the commuting case was similar enough to the classical setting that the classical algorithms could be literally translated to a quantum algorithm. However, the progress for the non-commuting case stalled, and no one could devise a provably working algorithm for the general non-commuting case. There, I also applied ideas that later turned out to be well connected to QSVT, which in turned resulted in the most efficient algorithm for that problem [Gil19, Chapter 7]. Quantum Gibbs sampling overcomes the major limitation of the quantum Lovász Local Lemma, which only promises reasonable running times for 'sparsely constrained" Hamiltonians, but comes with the next challenge, which is bounding the mixing times or discriminant spectral gaps.

Following our work on quantum Gibbs sampling [CKBG23, CKG23, GCDK24] we have several candidate algorithms for quantum Gibbs sampling, and the time is ripe to start comparing them and analysing their behaviour for specific systems of interest, e.g., coming from statistical physics or optimization in quantum semi-definite program (SDP) solving [vAGGdW20, vAG19]. A tantalising connection is that in nature, cooling processes are analogous to Gibbs sampling, where the system gradually reaches thermal equilibrium through random exchanges of energy. This natural phenomenon reflects how systems thermalise, implying that the mixing time—the time required for a system to approximate its equilibrium distribution—should be well-behaved for systems that naturally reach thermal equilibrium. Physics wisdom suggests that systems which efficiently thermalise in nature also exhibit favourable mixing times when modelled through Gibbs sampling, indicating an inherent efficiency in reaching equilibrium states. This insight is critical for understanding and predicting the behaviour of complex systems.

There are many similarities between the quantum Lovász Local Lemma and quantum Gibbs sampling: both can be viewed as dissipative algorithms, in the commuting case certain classical arguments can be nicely transferred to quantum case, and the generalization to the general non-commuting quantum case stalled before I started working on the problem. Since techniques and ideas related to the QSVT framework are very important for the efficient implementation of the arising general purpose algorithms I believe I have a well fitting background for finding promising efficient algorithms for quantum Gibbs sampling.

2 Research Summary

Markov Chain Monte Carlo (MCMC) methods, particularly the Metropolis algorithm and Glauber dynamics, are foundational techniques in statistical physics for simulating the behaviour of large, complex systems that have become indispensable across various fields, including computational physics, biology, and finance. These MCMC algorithms can sample from complex probability distributions making them crucial for tasks such as option pricing, risk management, and optimization problems in financial modelling. The core of the technique is a simple iterative process exploring the state space of a system through local updates, allowing for the approximation of the equilibrium distribution efficiently. The power of MCMC methods is that they effectively work with an exponentially large stochastic matrix and simulate its effect probabilistically without needing to explicitly apply matrix operations by choosing appropriate probabilistic transitions among basis states.

In the quantum case the goal is to sample from a distribution over quantum states, and a quantum computer in principle can apply a similar strategy designing appropriate transitions among quantum states – which can be a superposition of exponentially many basis states. In particular, the arising quantum algorithm can be used for simulating quantum physical systems, whose classical simulations are computationally infeasible for large systems, promising new insights to complex quantum mechanical systems. Quantum generalizations of MCMC methods, such as the Metropolis algorithm and Glauber dynamics, aim to leverage quantum superposition and entanglement to explore the state space more efficiently.

Previous attempts to generalize classical MCMC methods to quantum systems [TOV$^+$11, YAG12] encountered significant hurdles. The main obstacle was the inherent quantum uncertainty in learning properties of quantum states that would help executing the desired transitions or "jumps", and resulted in issues concerning non-locality and entanglement. Most importantly, these uncertainties led to difficulties in maintaining the detailed balance and efficient sampling, which are crucial for the success of these algorithms, and the proposals relied on subroutines that turned out to be provable impossible to implement [CKBG23, Appendix H]. However, recent advancements [CKBG23, CKG23, GCDK24], have identified a viable quantum generalization that mitigates these issues. The new breakthrough approach incorporates quantum transitions in a coherent fashion while preserving the desirable properties of the classical methods, in particular it maintain exact detailed balance. We plan to explore further generalizations, extensions and improvements over these first constructions.

Understanding the mixing times of these quantum algorithms is another critical step in obtaining efficient algorithms. A recent result [RSFA24] shows that for high enough temperature the process described in [CKG23] converges in polynomial time, which is the first known results in the general non-commuting case. The proof heavily relies on the detailed balanced properties of our construction, providing initial insights into the mixing time behavior of quantum MCMC algorithms, and uses a perturbative approach relating high-temperature dynamics to the basic infinite temperature dynamics. We plan to explore non-perturbative approaches to establish new comprehensive bounds and to understand the factors influencing the mixing times in different quantum systems. This could help understanding how to choose the jump or transition operators, and apply other system-specific fine-tuning of the general algorithms [GCDK24].

The successful development and understanding of quantum generalizations of MCMC methods could herald practical quantum algorithms for demonstrating a clear quantum advantage. By enabling simulations that are infeasible for classical computers, these algorithms could revolutionize various domains, from material science to financial modelling, offering unprecedented computational power. It could potentially also speed up quantum SDP solving, which is also based on Gibbs sampling [BS17], however for Hamiltonians that are related to the constraint matrices of the SDP rather than quantum physical systems. SDP's represent fairly general optimization problems, which are however limited in their applicability due to the costly matrix operations required for solving them. Yet, SDPs are popular because they come with provable guarantees on the quality of the solution. Thus, this research not only aims to advance the theoretical framework of quantum algorithms but also aspires to realize tangible benefits that underscore the transformative potential of quantum computing.

3 Connection to the highly successful classical MCMC paradigm

A major observation is that quantum mechanical thermal Lindbladians, in particular the so-called Davies generator, can be viewed as a continuous-time quantum variant of the classical Metropolis algorithm for sampling from the Gibbs distribution. In the Gibbs distribution the energy eigenstate ψ_i with energy E_i is present with probability proportional to $\exp(-E_i)$, where ψ_i is an eigenvector of the system Hamiltonian $\boldsymbol{H}$ with eigenvalue E_i (called the energy of the eigenstate ψ_i in physics). Despite the clear connection, early attempts at designing quantum MCMC algorithms have been compromised by obstacles rooted in quantum effects such as uncertainty relations, non-locality, and entanglement, which are especially problematic when the system Hamiltonian $\boldsymbol{H}$ consist of non-commuting local terms.

To highlight these obstacles consider the following Metropolis-style procedure: suppose we start with an energy eigenstate ψ_i and apply a jump A. If the energy decreases, we wish to "accept" this move; otherwise, we "reject" this move with a prescribed probability. However, this conflicts with the energy-time uncertainty principle (to know confidently whether energy has increased or decreased) and the no-cloning theorem (to return to the previous quantum state without keeping many copies). To tackle these obstacles prior work had to unrealistically assume perfect metrology (by either performing exponential time quantum phase estimation or assuming the Hamiltonian spectrum has artificial-looking periodic gaps); other works attempt to address both challenges simultaneously at the price of giving up other desirable analytic and algorithmic properties of classical MCMC algorithms: detailed balance is lost. We think that this is the primary reason why the potential impact of quantum MCMC algorithms has been largely under the shadows in the community.

We realized that the key reason behind the struggles of earlier attempts at designing quantum MCMC algorithms is that they aimed at devising a process that mimicks the textbook Davies generator, either directly or via some ill-behaved sharp discretization. However, it is well-known in the open systems community that the Davies generator has some non-physical features, e.g., it has some unrealistically rapid relaxation times for certain quantities and it depends non-continuously on the system Hamiltonian [GCDK24]. We believe that it is ultimately due to these non-physical aspects of the textbook Davies generator that hindered earlier simulation attempts.

Continous-time Markov Chains and detailed balance. To set the stage for Quantum MCMC algorithms, we review the key classical notions. A *continuos-time Markov chain* has an infinitesimal generator $\boldsymbol{L}$ of transitions on instantaneous probability distributions $p(t)$

$$\frac{\mathrm{d}p(t)}{\mathrm{d}t} = \boldsymbol{L}p(t), \tag{1}$$

and the effect of time-t evolution is described by the stochastic matrix $\mathrm{e}^{t\boldsymbol{L}}$.

The cornerstone of MCMC methods is *detailed balance*, which is a symmetry relation with respect to the distribution π requiring that the probability mass transfer between all pairs s, s' of configurations is equal in both directions

$$L_{s's}\pi_s = L_{ss'}\pi_{s'}, \quad \text{which then also ensures stationarity} \quad \boldsymbol{L}\pi = 0. \tag{2}$$

Remarkably, detailed balance gives a general recipe to *prescribe* any stationary state π that one wishes to sample from. Under reasonable assumptions [GCDK24], π can be ensured to be the *unique* stationary state, and thus the algorithmic cost to sample from the stationary state then simply scales with cost to simulate the time dynamics (per unit time $\mathrm{e}^{\boldsymbol{L}}$) multiplied by the convergence time (i.e., the mixing time). Detailed balance also ensures that the mixing time reduces to the *spectral gap* of the chain, a quantity amenable to numerical and analytic bounds. The above principle is manifested in Glauber dynamics [Gla63] (and the Metropolis algorithm [MRR$^+$53] as a discrete-time counterpart) for sampling Gibbs distribution $\pi \propto \mathrm{e}^{-H}$ of classical Ising Hamiltonians, where detailed balanced dynamics can be *implemented* efficiently and the mixing time can be fully characterized. To run the corresponding algorithm, the user merely needs to specify the Hamiltonian H, and a set of "jumps" (e.g., flipping spins randomly). The robustness and simplicity of the algorithm have led to a comprehensive understanding of phase transitions and thermal properties of classical magnets.

Lindbladians and quantum detailed balance. The natural quantum counterpart is a *continuous-time Quantum Markov chain* (a.k.a., Lindbladian, Liouvillian, or master equation) parametrised by a set of Krauss operators $\{\boldsymbol{K}_j\}$ and a Hamiltonian $\boldsymbol{B}$:

$$\frac{\mathrm{d}\boldsymbol{\rho}(t)}{\mathrm{d}t} = \mathcal{L}[\boldsymbol{\rho}(t)] := \underbrace{-\mathrm{i}[\boldsymbol{C}, \boldsymbol{\rho}(t)]}_{\text{“coherent”}} + \sum_j \underbrace{\boldsymbol{K}_j \boldsymbol{\rho}(t) \boldsymbol{K}_j^\dagger}_{\text{“transition”}} - \underbrace{\frac{1}{2}\Big(\boldsymbol{K}_j^\dagger \boldsymbol{K}_j \boldsymbol{\rho}(t) + \boldsymbol{\rho}(t) \boldsymbol{K}_j^\dagger \boldsymbol{K}_j\Big)}_{\text{“decay”}}. \tag{3}$$

The above generic form guarantees that the generated map $\mathrm{e}^{t\mathcal{L}}$ is a valid quantum Markov chain mapping density operators to density operators (called completely-positive-trace-preserving or CPTP operator).

Let $\boldsymbol{H}$ be an arbitrary *non-commuting* Hamiltonians $\boldsymbol{H} = \sum_i E_i |\psi\rangle\langle\psi_i|$ with (potentially unknown) eigenstates. The *quantum detailed balance* condition (QDB) with respect to the mixed-state $\boldsymbol{\rho} \propto \mathrm{e}^{-\boldsymbol{H}}$ is

$$\mathrm{e}^{-(E_1+E_2-E_1'-E_2')/2} \langle\psi_1'|\mathcal{L}[|\psi_1\rangle\langle\psi_2|]|\psi_2'\rangle = (\langle\psi_1|\mathcal{L}[|\psi_1'\rangle\langle\psi_2'|]|\psi_2\rangle)^* \tag{4}$$

which then also ensures stationarity of the Gibbs state, i.e., $\mathcal{L}[\boldsymbol{\rho}] = 0$.

The quantum state during the dynamics can be mixture of superpositions of different energy eigenstates, and quantum detailed balance (4) requires the transition amplitudes between pairs of energy eigenstates to be related by a certain Boltzmann factor of the average of energy differences $E_1 - E_1'$ and $E_2 - E_2'$.

Davies generators – the prototype of quantum detailed balance. In 1976, Davies derived a Lindbladian from first principles by considering a physical system interacting with a large thermal bath under a weak-coupling and infinite-time limit. The Lindblad operators in Davies' generator are given by certain Fourier transform of Heisenberg dynamics, which with a bit of hand-waving can be written as

$$\boldsymbol{K}_\nu = \sqrt{\gamma(\nu)} \sum_{\substack{E_i, E_j \\ E_i - E_j = \nu}} \langle\psi_1|\boldsymbol{A}|\psi_2\rangle |\psi_1\rangle\langle\psi_2| \tag{5}$$

$$\propto \sqrt{\gamma(\nu)} \int_{-\infty}^{\infty} \mathrm{e}^{\mathrm{i}\boldsymbol{H}t} \boldsymbol{A} \mathrm{e}^{-\mathrm{i}\boldsymbol{H}t} \mathrm{e}^{-\mathrm{i}\nu t} \mathrm{d}t \tag{6}$$

of certain $\boldsymbol{A}$ are “jump operators” through which the system is connected to the bath (e.g., local Pauli operators), and ν is a *Bohr frequency*, i.e., an energy difference between two eigenstates. Colloquially, $\boldsymbol{K}_\nu$ contains “the part of transition amplitudes in $\boldsymbol{A}$ that changes the energy by ν”, which is precisely what the above operator Fourier transform diagnoses.

The function $\gamma(\nu)$ are tunable transitions weights, reminiscent of classical Glauber dynamics. Quantum detailed balance is automatically satisfied whenever $\gamma(-\nu) = \mathrm{e}^{-\nu}\gamma(\nu)$ holds. Intuitively speaking we should favour cooling (the energy decreases $\nu < 0$) and exponentially suppress heating (the energy increases $\nu > 0$). Conceptually, the Davies map can be considered a natural quantum extension of Glauber dynamics as it satisfies quantum detailed balance with respect to the Gibbs state. Moreover, for a classical Ising Hamiltonian, when the input state is classical and the jumps $\boldsymbol{A}$ are classical spin flips, the Davies map recovers the classical Glauber dynamics.

The critical problem with the Davies' generator is the infinite time integral over an arbitrarily long Hamiltonian evolution, which is the root-cause of the aforementioned unphysical discontinuous properties. From an implementation perspective, the integral can be truncated at a time-scale inversely proportional to energy level-spacing, however it is only tractable for small quantum systems (e.g., in quantum optics) or commuting Hamiltonians. Unfortunately, for non-commuting many-body problems where the energy levels are exponentially close, the Davies' generator cannot be implemented efficiently and perhaps do not even capture many-body systems in the thermodynamic limit.

Restoring quantum detailed balance and locality. What appears uncomfortable is the fact that quantum detailed balance refers to the exact energies and energy eigenstates while quantum metrology is intrinsically costly. In contrast, classical detailed balance has never been an issue since each configuration can be efficiently described (unlike quantum eigenstates) and take a definite energy value (unlike the

uncertainty principle for quantum observables). Unfortunately, despite several attempts [TOV$^+$11, YAG12, WT23], up until now, it was not known how to construct a mathematically simple Lindbladian that satisfies quantum detailed balance exactly, and for which $\boldsymbol{K}_j$ can be applied efficiently with a controllable error.

We proposed two modifications to the Davies generator that fixed all previous problems simultaneously [CKG23]. The first modification was to add a Gaussian damping term to the Fourier integral in (6), and the second modification was to choose the coherent term in (3) to restore detailed balance. The main observation was that choosing the Gaussian damping and the function γ appropriately results in detailed balances transitions. However, there is no particular reason for the resulting decay term to commute with the Gibbs state ρ, which is a uniquely quantum issue threatening detailed balance. Nevertheless, the remedy also comes from the uniquely quantum degree of freedom in choosing the coherent term, providing an essentially unique fix [CKG23]. Combining these ideas we constructed the first quantum MCMC algorithm that satisfies *detailed balanced* yet have *efficiently implementable* dynamics – the efficiency and the locality of the transitions being a direct consequence of the exponential damping of the Gaussian, see [CKG23].

While the existence of an exactly detailed balance Lindbladian might seem little more that a curiosity, it in fact has profound algorithmic implications. Most importantly, the jump operators have a fixed damping rate $\Theta(1)$ independent of the mixing time[CKG23, GCDK24]. This means that the Hamiltonian evolution needs only be performed for a time proportional to $\Theta(1)$, and the integral truncation error is controlled. Since the invention of this first construction, some alternative constructions have been devised [DLL24, GCDK24] generalising the above recipe.

4 Open questions to be addressed and research timeline

In light of the above described recent developments I list some major open problems that I would like to tackle in the context of this research proposal.

General techniques for mixing time bounds in the non-commuting case. One of the most pressing open problem is to understand mixing times of our quantum Gibbs samplers. There are several ways to approach this problem. First, it is worth to try and adapt the perturbation technique that was successfully applied for analysing the construction of [CKG23] to the newer constructions of [DLL24, GCDK24]. Second, the approaches based on logarithmic Sobolev inequalities [CRSF21] that were successfully applied to several commuting systems should be examined in the non-commuting context regarding the constructions [CKG23, DLL24, GCDK24]. Finally, we shall revisit classical mixing-time bounding techniques based on for example coupling methods [BRO23], that might be applicable in the quantum context as well.

Study of the corresponding discrete-time algorithms. Form an analytic perspective the continuous-time quantum process appears to be more clean, however the recently devised discrete-time counterparts [GCDK24] can be advantageous from an implementation perspective. Therefore, it is important to understand, to what extend can we relate the mixing-times of the continuous- and discrete-time variants.

Study of geometrically local systems. Based on the general techniques we intend to study spin systems and other physically motivated quantum systems, which are expected to thermalise, i.e., where physics wisdom suggest the mixing times should be nicely bounded. For one dimensional systems we expect rapid mixing, and we hope this could be proved using an argument motivated by the renormalization group approach [ALVV17]. After studying the one dimensional case we will try and see which techniques generalize to higher dimensions. While studying particular systems we evaluate the need for specific jump operators via tensor-network simulations, and modify the algorithm and analytic proofs accordingly.

Purified Gibbs state preparation. The mixing time can be directly related to the spectral gap of the discriminant matrix [CKBG23]. Moreover, if there is a continuous path of discriminants connecting the current discriminant to a trivial one, then we can use a variant of the adiabatic algorithm to prepare a purification of the Gibbs state [CKBG23]. We shall study what happens at phase transitions, and whether there are instances when a rapidly mixing region seems unreachable by such an adiabatic path.

Gibbs states coming from SDP solvers. Quantum Gibbs sampling is known to be QMA-hard in general, therefore we do not expect the mixing time to be generally small. However, it is worth studying if for some particular class of SDPs there are some performance guarantees that enable speeding up quantum SDP solving via our new Gibbs samplers. This is essentially known for sparse random constraint matrices [CDB+24], however we shall be looking out to find examples that are more relevant in practice.

Research Problems	Year 1	Year 2	Year 3	Year 4
General mixing time bounds	perturbative	log-Soboliev	coupling	discrete-time
Geometrically local systems	1D lattice	$\geq$ 2D lattice		
Purified Gibbs state prep.			1D lattice	$\geq$ 2D lattice
Gibbs states in SDP solvers	awareness	awareness	awareness	awareness

Table 1: Research proposal timeline. The main objective is to study generic mixing time bounds which is spanning the entire 4 years, and the table indicates which particular approach would be the focus in the given year of the proposal. In the final year we intend to study which of the approaches that worked in the continuous-time setting could be adapted to the discrete-time case. In parallel to the generic bounds in the first two years we intend to study particular (Ising) spin systems that feature a 1 or higher dimensional geometric lattice structure. In the last two years we plan to study the problem of preparing purified Gibbs states and the associated problem of the discriminant gap in lattice systems. While we work out the details of these methods and systems we shall keep an eye on classic SPD problems such as the MAX-CUT relaxation to see if the currently studied mixing-time bounds give any promise on the performance of the associated quantum Gibbs sampler. We plan to publish an article related to each of the first 4 open problems, and potentially also about SDP solvers if we find a promising candidate problem.

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[YAG12] Man-Hong Yung and Alán Aspuru-Guzik. A quantum-quantum Metropolis algorithm. *Proceedings of the National Academy of Sciences*, 109(3):754–759, 2012. arXiv: 1011.1468

Participating researchers

João Doriguello is a highly qualified candidate for this quantum algorithms research project. He is currently a postdoctoral researcher at the HUN-REN Alfréd Rényi Institute of Mathematics. He has extensive experience in quantum computing, having held a postdoctoral positions at the Centre for Quantum Technologies in Singapore where he worked with Miklós Sántha after completing his PhD studies at the University of Bristol under the supervision of Ashley Montanaro. His research interests include query complexity, quantum finance, and quantum algorithms in general. João has a robust publication record, with works on quantum algorithms for machine learning, optimization and finance. His broad expertise and innovative research make him an excellent fit for this research project especially considering that we already coauthor a manuscript on a precursor of this project [GCDK24]. The intention is to involve him with an average 0.2 FTE in the project, and he would primarily work on estimating mixing times and trying to find further quantum variants potentially covering the non-self-adjoint case which is analogous to the Hastings' generalization [Has70] of the Metropolis algorithm [MRR$^+$53].

Balázs Kabella is a highly talented and motivated candidate who just applied for a PhD position under my supervision at the Eötvös University's Computer Science Faculty. He developed a deep expertise in tensor network theory during his master's studies at the University of Manchester. As a matter of fact we already started working on a related research project where he is developing novel classical simulation methods inspired by our quantum algorithms for sampling Gibbs states. These methods promise significant advancements in simulating many-body quantum systems, and Balázs playing a pivotal role in the project. His maturity in research, coupled with his meticulous, precise, and innovative approach, demonstrates his exceptional scientific potential and technical skills, making him an outstanding fit for advanced research in quantum Metropolis sampling. I plan to involve him in the research from a numerical angle with 0.4 FTE. His simulations could deliver important intuitive understanding of mixing times, supporting the analytic studies. Also the simulations are expected to provide insights on how to choose the "jump" operators for various physical systems of interest. After understanding and distilling the numerical results he would also take part in the derivation of analytic proofs supported by the gained intuition.

Research capacity devoted to this project

Name	Participation time	Senior	2025-01-01 - 2025-12-31	2026-01-01 - 2026-12-31	2027-01-01 - 2027-12-31	2028-01-01 - 2028-12-31	FTE
			FTE				
Gilyén András	2025-01-01 - 2028-12-31	✓	0.40	0.40	0.40	0.40	1.60
Total							1.60

Participants', list of publications and citations, scientometrics

Gilyén, András Curriculum vitae

Degree

Year of PhD	2019
University/Institution	University of Amsterdam
PhD registration number	19532
Title of the PhD dissertation	Quantum Singular Value Transformation & Its Algorithmic Applications

Languages

English	**Advanced Level Write and read (C)**

Qualifications

2013	**Master of Advanced Studies, Cambridge**
2014	**MSc Mathematician, Eötvös University**

Decorations

2019	**Best student paper award** *by*: Track A of the 46th International Colloquium on Automata, Languages, and Programming (ICALP) *Achievement*: Paper: Improvements in Quantum SDP-Solving with Applications
2019	**Cor Baayen Young Researcher Award** *by*: European Research Consortium for Informatics and Mathematics *Achievement*: PhD thesis and young researcher's track record
2021	**Junior Prima Award** *by*: Prima Primissima Foundation & Hungarian Development Bank *Achievement*: young researcher's track record

Study trips - stipends

2017 (3 Month)	**Quantum Architectures and Computation Group, Microsoft Research** *Sponsor*: Microsoft Research *Research topic*: Research intern
2020 (3 Month)	**Simons Institute for the Theory of Computing, UC Berkeley** *Sponsor*: Google *Research topic*: Research Fellow at “The Quantum Wave in Computing” Program

Role in scientific community

2021 - 2022	**Program committee member of the Annual Conference on Quantum Information Processing (QIP)**
2023 - 2023	**Program committee member of the 64th Annual Symposium on Foundations of Computer Science (FOCS)**

Workplaces

2014 - 2015 **Quantum Optics and Quantum Informatics Department (Wigner Research Centre for Physics)**
Position: Tudományos segédmunkatárs

2015 - 2019 **Centrum Wiskunde & Informatica**
Position: PhD student

2019 - 2021 **California Institute of Technology**
Position: postdoc

2021 - **(Alfréd Rényi Institute of Mathematics)**
Position: research fellow

Relevant publications published in the last five years

Publication or achievement	Impact	Number of citations
van Apeldoorn Joran, Cornelissen Arjan, Gilyén András, Nannicini Giacomo: ***Quantum tomography using state-preparation unitaries***, In: Nagarajan, Viswanath; Bansal, Nikhil (szerk.) Proceedings of the 2023 Annual ACM-SIAM Symposium on Discrete Algorithms (SODA), Society for Industrial and Applied Mathematics (2023) pp. 1265-1318., 2023; doi:10.1137/1.9781611977554.ch47 *	-	22
Chia Nai-Hui, Gilyen Andras Pal, Li Tongyang, Lin Han-Hsuan, Tang Ewin, Wang Chunhao: ***Sampling-based Sublinear Low-rank Matrix Arithmetic Framework for Dequantizing Quantum Machine Learning***, JOURNAL OF THE ACM 69: (5) 33, 2022; doi:10.1145/3549524; Research field: Artificial Intelligence ; position: 14/276 (D1) (Scopus ranking: journal position/length of list) *	-	52
Gilyén A., Song Z., Tang E.: ***An improved quantum-inspired algorithm for linear regression***, QUANTUM 6: 754, 2022; doi:10.22331/Q-2022-06-30-754; Research field: Atomic and Molecular Physics, and Optics ; position: 12/199 (D1) (Scopus ranking: journal position/length of list) *	-	23
Gilyén A., Hastings M.B., Vazirani U.: ***(Sub)Exponential advantage of adiabatic Quantum computation with no sign problem***, In: Khuller, S.; Williams, V.V. (szerk.) 53rd Annual ACM SIGACT Symposium on Theory of Computing, STOC 2021, Association for Computing Machinery (ACM) (2021) pp. 1357-1369., 2021; doi:10.1145/3406325.3451060 *	-	20
Ambainis A., Gilyén A., Jeffery S., Kokainis M.: ***Quadratic speedup for finding marked vertices by quantum walks***, In: Chuzhoy, J.; Kamath, G.; Tulsiani, M.; Makarychev, Y.; Makarychev, K. (szerk.) 52nd Annual ACM SIGACT Symposium on Theory of Computing, STOC 2020, Association for Computing Machinery (ACM) (2020) pp. 412-424., 2020; doi:10.1145/3357713.3384252 *	-	30
Ben-David S., Childs A.M., Gilyen A., Kretschmer W., Podder S., Wang D.: ***Symmetries, graph properties, and quantum speedups***, In: IEEE (szerk.) 2020 IEEE 61st Annual Symposium on Foundations of Computer Science (FOCS), IEEE (2020) pp. 649-660., 2020; doi:10.1109/FOCS46700.2020.00066 *	-	14
van Apeldoorn J., Gilyén A., Gribling S., de Wolf R.: ***Quantum SDP-Solvers: Better upper and lower bounds***, QUANTUM 4: p. 230., 2020; doi:10.22331/q-2020-02-14-230; Research field: Atomic and Molecular Physics, and Optics ; position: 9/183 (D1) (Scopus ranking: journal position/length of list) *	-	49
van Apeldoorn J., Gilyén A., Gribling S., de Wolf R.: ***Convex optimization using quantum oracles***, QUANTUM 4: p. 220., 2020; doi:10.22331/q-2020-01-13-220; Research field: Atomic and Molecular Physics, and Optics ; position: 9/183 (D1) (Scopus ranking: journal position/length of list) *	-	40
Gilyén A., Arunachalam S., Wiebe N.: ***Optimizing quantum optimization algorithms via faster quantum gradient computation***, In: 30th Annual ACM-SIAM Symposium on Discrete Algorithms, SODA 2019, Association for Computing Machinery (ACM) (2019) pp. 1425-1444., 2019; doi:10.1137/1.9781611975482.87 *	-	56
Gilyén A., Su Y., Low G.H., Wiebe N.: ***Quantum singular value transformation and beyond: Exponential improvements for quantum matrix arithmetics***, In: Charikar, M.; Cohen, E. (szerk.) STOC 2019 Proceedings of the 51st Annual ACM SIGACT Symposium on Theory of Computing, Association for Computing Machinery (ACM) (2019) pp. 193-204., 2019; doi:10.1145/3313276.3316366 *	-	273

* : It is transferred from a publication database

Summary of scientific productivity

Number of publications	In Hungarian	Not in Hungarian (published in Hungary)	Not in Hungarian (published abroad)	Total
Article in periodical			9	9
Article in periodical in SCI/WoS			9	9
Article in periodical in SCI/WoS first author			3	3
Article in periodical in SCI/WoS last author				
Book				
Monograph, critical edition, edition of primary source				
Chapter				
Conference proceedings		2	12	14
Patent				
Other	1	2		3
Total	1	4	21	26

Imported from MTMT database (MTMT) : 2024-06-18 (Gilyén András Pál)

Scientometric data	In the last 10 years	Total
Number of independent citations	990	990
Independent citations in SCI/WoS & Scopus	914	914
Number of journal articles in the first quarter (Q1) of the journal ranking list of the discipline	8	8
Number of journal articles in the top 10% (D1) of the journal ranking list of the discipline	7	7

Imported from MTMT database (MTMT) :
2024-06-18 (Gilyén András Pál)

Impact factor in the last 5 years (by own admission)	

Tasks of the participants

Gilyén András			(Alfréd Rényi Institute of Mathematics)
FTE:	1.60	Scientific tasks:	Research supervision, supervision of PhD students, mentoring of postdoctoral researchers.

Other ongoing research projects and submitted proposals by the senior participants

H2020

(QuantERA II ERA-NET Cofund in Quantum Technologies The Wigner Institute is the main node from Hungary, and Zoltán Zimborás is the lead researcher from the Hungarian side.)

Principal investigator	Participant in this proposal	FTE
Andris Ambainis	Gilyén, András	0.30

Title: Hybrid Quantum-Classical Computation

Project identifier	Number of participants	Amount of support (HUF)	Starting year	Closing year
HQCC-101017733	4	54000000	2022-09-01	2025-08-31

Summary:

Hybrid quantum-classical computing combines the power of quantum and classical processors to compute faster. This is of particular relevance in the current Noisy Intermediate-Scale Quantum (NISQ) computing era, when quantum processors are still very limited. Moreover, hybrid computing bears the strongest potential for reaching a practical quantum advantage, as it will take a long time before fault-tolerant quantum computers completely replace classical machines, if ever. For these reasons, hybrid quantum-classical architectures have taken center stage in the recent heuristic exploration of the potential of quantum computers. A rigorous framework is, however, painfully lacking to date. The goal of project HQCC is to put this important field onto solid theoretical footing. We aim to address the fundamental questions about the power of hybrid computation: – What problems are more amenable to the hybrid quantum-classical approach? – With what algorithms can we solve them? – What data structures and encodings perform better under this approach? – Can we classify how hard these problems are in this context, namely can we define hybrid quantum-classical computational complexity classes? To address these questions, project HQCC is structured into three complementary parts: one dealing with complexity-theoretic aspects (such as the regimes in which quantum advantage is possible), one concerned with algorithms for hybrid computation (for example, variational quantum algorithms and the most efficient ways to encode data into them), and one dealing with learning and training processes. These three components will be developed in dialogue with each other to extract a comprehensive understanding of hybrid quantum-classical computation. CONSORTIUM Coordinator: Andris Ambainis (Latvijas Universitate, LV) Jens Eisert (Freie Universität Berlin, DE) Zoltán Zimborás (Wigner Research Centre for Physics, HU) Yasser Omar (Associação do Instituto Superior Técnico para a Investigação e Desenvolvimento, PT)

Other International

(HORIZON-EIC-2024-PATHFINDEROPEN-01 Under review, support has not yet been granted. The topic is related to Lindblad simulation and mixing time estimation for the special case of magnetic systems.)

Principal investigator	Participant in this proposal	FTE
Frank Neese	Gilyén, András	0.60

Title: Advancing Magnetic Materials Simulation with Classical and Quantum Computation

Project identifier	Number of participants	Amount of support (HUF)	Starting year	Closing year
Magcomp-101187203	17	155000000	2025-01-01	2027-12-31

Summary:

Magnetic materials are used in various applications, from electric motors and generators to electronics such as hard drives and actuators. The lack of alternative materials or understanding of material recycling has resulted in an overdependence on limited geopolitically risky sources for the key rare earth metals required. This is a key challenge because high performance magnets are needed for both the net zero and digital transformations. Existing R&D is held back by shortcomings in simulation techniques which limit the speed with which new materials can be developed. Innovation breakthrough: This project aims to advance magnetic material simulation across multiple domains. Within classical simulation we aim to advance existing approaches by building up from the smallest building blocks of ab initio quantum simulation, using state-of-the-art ligand field theory and tensor network approaches. Within quantum computation we will tackle the major challenges of efficient initial state preparation, as well as going beyond existing work through the calculation of macroscopic properties from Green's functions. This will be accompanied by relevant benchmarking and resource estimation to enable realistic costings and the development of algorithms applicable to hardware that will be available within the next 10 years. Innovation potential: Several members of our consortium have already commercialised materials simulation code. Our objective is to create a toolbox that encompasses new advances in both classical and quantum computational approaches, focusing on end-user challenges to deliver valuable new tools for the magnetic materials simulation community across both academic and industrial users. Consortium: Magcomp brings together top academic researchers within classical and quantum computation fields, with an up-and-coming SME in the quantum computing field, as well as the applied computation expertise of a national HPC centre.

H2020 (Marie Curie Fellowship, with the main topic being the development of various quantum algorithms with no specific relation to quantum MCMC methods)				
Principal investigator	Participant in this proposal		FTE	
Gilyén András	Gilyén, András		2.00	
Title: Finding Order in Large-scale Structures by Quantum Computing				
Project identifier	Number of participants	Amount of support (HUF)	Starting year	Closing year
QuantOrder-891889	1	55000000	2021-09-01	2025-08-31

Summary:
Quantum computing is an emerging, interdisciplinary field of science in the intersection of computer science, mathematics and physics. Recent experimental advances in building a physical quantum computer show the urgency of finding possible applications. On the other hand to date we only have very small quantum computers, which are mostly useful for proof of concept demonstrations, thus for the time being one needs to focus on building and understanding the underlying mathematical theory. A particularly interesting aspect of quantum computing is quantum machine learning, which also needs a more firm theoretical understanding, because many of the recent developments are based on heuristic approaches which cannot be properly tested yet, due to the limitations of the available hardware. This proposal outlines new approaches and ideas for quantum algorithm development, and attempts to improve some aspects of the theory of quantum machine learning, while also encompasses some fundamental theoretical questions. The described ideas are all related to the problem of finding large-scale structures in various objects. Since quantum computers tend to be quite efficient at recognizing patterns, it is a promising angle of approach. The relevant ideas are inspired by multiple related disciplines, and several of the proposed tools were recently co-developed by the applicant. The supervisor has an outstanding track record in developing the mathematical theory of large-scale structures emerging in graphs, groups and networks, while the applicant has demonstrated strong problem solving skills and the ability of developing novel quantum algorithms, which promises a fruitful collaboration in the implementation of the proposed action.

Other International (Amazon-sponsored research, there is an overlap in the topic of Lindblad simulation.)				
Principal investigator	Participant in this proposal		FTE	
Gilyén András	Gilyén, András		0.40	
Title: Quantum Singularity II				
Project identifier	Number of participants	Amount of support (HUF)	Starting year	Closing year
AWS-CQC-II	1	50000000	2023-09-01	2024-08-31

Summary:
Joint research with Amazon Web Services, in collaboration with their quantum algorithms team. The main topic is the development of new and practically applicable quantum algorithms.

NKFI	Principal investigator: **Gilyén, András**	Identifier: **151294**	**STARTING**	Version: **2**	9. Section

Closed OTKA/NKFIH projects' details

Project identifier	Principal investigator	Starting year	Closing year	
124351	Kiss, Tamás	2017-09-01	2022-12-31	10 (excellent)
Title: Dynamics and measurement in coherent and open quantum information networks				

Budget table

NKFI registration number:			
Identifier:	151294		
Principal investigator:	Gilyén, András		
Title:	Quantum Generalizations of Markov Chain Monte Carlo Methods		
Institution:	(Alfréd Rényi Institute of Mathematics)		
Duration:	48	Duration:	2025-01-01 - 2028-12-31

	Cost (in Forint)	2025.01.01 -2025.12.31	2026.01.01 -2026.12.31	2027.01.01 -2027.12.31	2028.01.01 -2028.12.31	Total
1	Personnel	8 688 000	8 718 000	8 733 000	8 748 000	34 887 000
2	Travel and consumables	2 600 000	2 600 000	2 600 000	2 600 000	10 400 000
3	Overhead	2 357 000	2 323 000	2 276 000	2 279 000	9 235 000
4	Operational costs (1+2+3)	13 645 000	13 641 000	13 609 000	13 627 000	54 522 000
5	Equipment	500 000	300 000	50 000	50 000	900 000
6	Total costs (1+2+3+5)	14 145 000	13 941 000	13 659 000	13 677 000	55 422 000

Justification of personnel costs
For the principal investigator, I calculated the salary and benefits proportional to 0.4 FTE based on their research classification. In total, I accounted for 2 researchers, including 1 postdoctoral researcher and 1 PhD student, who will receive partial salary payments. The per diem allowances are also planned in this line, calculated at 80 euros per day for researchers' foreign stays (e.g., conferences, professional meetings) at an exchange rate of 400 HUF/euro, and I have included the taxes payable on these payments according to current regulations (13% social contribution tax).
Justification of travel and consumable costs
The travel costs associated with professional trips (e.g., conference participation, professional consultations, accommodation for invited researchers, and domestic travel expenses) have been planned. This includes expenses such as airfare, accommodation fees, registration fees, and foreign public transportation, as well as coverage for other material costs during the stay. Additionally, the procurement of other low-value office supplies (copy paper, toner) has also been accounted for.
Justification of equipment costs
The necessary equipment for the researchers to implement the project (computing devices, 1 laptop, 1 tablet) has been planned.