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Executive summary

The NISQ project ("Near-term quantum computers: challenges, optimal implementations and applications") has been established to characterize the computational power and to investigate possible practical applications of quantum computing devices consisting of a limited number of imperfect qubits. The Quantum Error Correction Group in NISQ aims at developing new techniques to cope with noise and imperfections affecting quantum systems from physically motivated interactions with realistic environments using techniques of statistical physics and open quantum systems.

Background and prior work

Previous work by the Group Leader was based on the path-integral approach to open quantum systems pioneered by Feynman and Vernon[1]. This starts from the transition probability $P_{if} = \mathrm{Tr}_B \langle f|U\left(|i\rangle\langle i| \oplus \rho_B^{eq}\right)U^{\dagger}|f\rangle$ of an open quantum system to develop from state i to state f, while interacting with a bath through the unitary operator U. The initial state of the bath is an equilibrium density matrix ρ_B^{eq}. The interaction is assumed linear and the bath energy quadratic in the bath coordinates and momenta. Important physical thermal environments (phonons, photons) can be represented as such harmonic oscillator baths, which can then be integrated out. What remains is a double integral over "forward" and "backward" system paths, which encode both the system parts of U and $U^{\dagger}$, and interference terms between the two paths known as the Feynman-Vernon action. The kernels of those interference terms can be identified with bath correlation functions, as is also known from Keldysh theory[2]. Alternatively, the Feynman-Vernon theory can be derived by an analysis of the von Neumann-Liouville equation[3].

Quantum annealing are restricted classes of algorithms that rely on a family of Hamiltonians expressed in terms of $\hat{\sigma}_z$ operators acting on some qubits. These families interpolate between a simple problem (say, linear in all $\hat{\sigma}_z$) and a complicated one of interest (say, polynomials in $\hat{\sigma}_z$ which encode a classical optimization problem). The process starts with the system of qubits in the ground state of the simple problem. To this Hamiltonian is added linear terms in $\hat{\sigma}_x$ that describe quantum tunneling; if the interpolation is done

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[1] R.P Feynman and F.L Vernon. "The theory of a general quantum system interacting with a linear dissipative system". In: *Annals of Physics* 24 (1963).

[2] Alex Kamenev. *Field Theory of Non-Equilibrium Systems.* Cambridge University Press, 2011.

[3] Erik Aurell, Ryoichi Kawai, and Ketan Goyal. *An operator derivation of the Feynman-Vernon theory, with applications to the generating function of bath energy changes and to anharmonic baths.* arXiv:1907.02671. 2019.

slowly enough the system will then end up in the ground state of the complicated system. The performance of quantum annealing algorithms have been analyzed by many groups[4].

If the qubits also interact with a harmonic oscillator environment, the evolution of the their state is described by Feynman-Vernon theory if the evolution of the qubits themselves are described by path integrals. For qubits interacting with themselves as in quantum annealing such paths can be piece-wise constant up or down, as introduced by Leggett and collaborators for the spin-boson problem[5]. For qubits interacting in a more general manner than quantum annealing one can start from a general path integrals for spins[6] which were used to analyze errors in quantum computing in[7].

The Feynman-Vernon theory gives the quantum map for the evolution of a mixed state interacting with a given environment, in itself a complicated object, which often needs to be approximated. The benchmark of all theories of open quantum systems are Quantum Markov Equations (Lindblad Equations). Interactions with a harmonic oscillator bath lead to Quantum Markov Equations when the system-bath terms are weak and driving is slow[8], so that, in comparison, the Feynman-Vernon kernels can be considered memory-less. This is appropriate for many problems, but not for quantum computing applications at very low temperature, since the bath correlation function memory time will then be long.

The spin-boson problem (quantum annealing with one qubit) has motivated a very large literature. One main alternative to Quantum Markov Equations is to assume that the tunneling terms (the $\hat{\sigma}_x$ terms in above) are small. This leads to the "non-interacting blip approximation (NIBA)" (Leggett et al 1987, *op cit*), which can be extended to a set of qubits interacting with a bath in this manner. For qubits interacting with themselves in a more general way a simple approximation like NIBA does not exist at this point. For more detailed analysis Feynman-Vernon theory can be approximated numerically by averaging over a set of fictitious random fields representing the bath correlation functions[9], or by the hierarchical equation of motion approach[10]. The latter assumes that bath correlation functions can be approximated by a few exponentials, which for simple baths in turn implies high enough temperature, but allow for a fast drive. Both of these methods are in principle quite general, but do not scale very well to large systems.

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[4] Victor Bapst et al. "The Quantum Adiabatic Algorithm applied to random optimization problems: the quantum spin glass perspective". In: *Physics Reports* 523 (2013).

[5] A. J. Leggett et al. "Dynamics of the dissipative two-state system". In: *Rev. Mod. Phys.* 59 (1 Jan. 1987), pp. 1–85.

[6] Alexander Atland and Ben Simons. *Condensed Matter Field Theory.* Cambridge University Press, 2006.

[7] Erik Aurell. "Global Estimates of Errors in Quantum Computation by the Feynman–Vernon Formalism". In: *Journal of Statistical Physics* 171 (2018), p. 745.

[8] Ulrich Weiss. *Quantum Dissipative Systems, 4th Ed.* World Scientific, 2012.

[9] Jürgen T. Stockburger and C. H. Mak. "Stochastic Liouvillian algorithm to simulate dissipative quantum dynamics with arbitrary precision". In: *J. Chem. Phys.* 110 (1999), p. 4983.

[10] Akihito Kato and Yoshitaka Tanimura. "Hierarchical Equations of Motion Approach to Quantum Thermodynamics". In: *Thermodynamics in the Quantum Regime: Fundamental Aspects and New Directions.* Ed. by Felix Binder et al. Cham: Springer International Publishing, 2018, pp. 579–595.

Near- and long-term research projects in NISQ

The generating function for energy changes in a bath is defined as

$$G_{if}(\nu) = \mathrm{Tr}_B \, \langle f| e^{i\nu H_B} U e^{-i\nu H_B} \left(|i\rangle\langle i| \oplus \rho_B^{eq}\right) U^\dagger |f\rangle$$

where the parameter ν sets the scale of the bath energy change. For $\nu = 0$ this is the same as the Feynman-Vernon transition probability P_{if}. Similarly to that case, the bath can be integrated out when it consists of harmonic oscillators. This is the project started in[11], with the outcome that $G_{if}(\nu)$ is practically the same as P_{if}, with only a time shift in the influence functional terms coupling the forward and backward paths[12]. The result follows more simply in the approach of (Aurell, Kawai and Goyal 2019 *op cit*), where the system and baths are coupled as $X_S \otimes Y_B$, and the Feynman-Vernon kernels are the unequal-time pair-correlations of the Y_B operators in the unperturbed bath. For harmonic oscillator baths all correlations can be expressed in pair-correlations (Wick's theorem), but in general there will be corrections (non-zero cumulants). A second result in (Aurell, Kawai and Goyal 2019 *op cit*) is that such cumulants translate to explicit higher-than-quadratic terms in the Feynman-Vernon action.

First project, near-term, is to follow up on this last development in concrete examples. One goal is to look for new ways to estimate the development of a qubit or a few qubits interacting with a "spin bath"[13]. This is on the assumption that at very low temperatures the most important excitations in a material are not delocalized phonons, but localized impurities. A second goal is to consider baths of conduction band electrons, in normal metals. Such fermionic degrees of freedom can interact with a macroscopic quantum state similarly to the Frölich polaron model (quadratic in the fermions), a case that can also be analyzed by the method in (Aurell, Kawai and Goyal 2019 *op cit*). This is particularly interesting in the context of quantum heat flows, since the leading experiments on quantum heat flows through small superconducting circuits are built on these principles[14]. What one calls noise in quantum systems is physically the effects of interactions with an unobserved and uncontrolled environment. Overall, this first project hence addresses the NISQ goal to develop new techniques to cope with noise.

Second project, also near-term, is to study large deviations, that is the distribution of large but rare events. Mathematically (and classically), large deviations is the method of choice to study imperfections and their effects, by estimating the asymptotic behavior of tails of probability distributions. Applications can be found in in statistics, in information and communication theory, in finance and insurance mathematics (ruin theory), and in many engineering fields. Large deviations of quantum particle and heat currents were first

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[11] Erik Aurell and Ralf Eichhorn. "On the von Neumann entropy of a bath linearly coupled to a driven quantum system". In: *New Journal of Physics* 17.6 (2015), p. 065007.

[12] Erik Aurell. "A simplified characteristic functions of quantum heat". In: *arXiv* (2019), p. 1904.03496.

[13] N V Prokof'ev and P C E Stamp. "Theory of the spin bath". In: *Reports on Progress in Physics* 63.4 (2000), p. 669.

[14] Alberto Ronzani et al. "Tunable photonic heat transport in a quantum heat valve". In: *Nature Physics* 14 (10 2018), pp. 991–995.

studied about ten years ago in a fairly abstract setting, *e.g.* to prove Gallavotti-Cohen theorems[15]. Beginning slightly later quantum large deviations have also been studied in concrete examples by Garrahan and co-workers[16], but (so far) only for Quantum Markov Processes. An immediate goal is to extend the results in (Aurell & Montana 2019 *op cit*) from thermal power (expected heat per unit time) to the full rate equation, within the NIBA approximation. Large deviations of heat and particle number currents is one of the major themes of modern non-equilibrium statistical physics, and it is an exciting prospect that we can also address that on the quantum level, for spin-boson problems and their generalizations, and also beyond weak-coupling approximations.

Third project, intermediate term, is motivated by the fact that all computation must generate heat according to Landauer's principle. For controlled over-damped diffusion processes we found some years ago a universal correction to Landauer's which is inversely proportional to duration of the process[17]. This means that if bit erasure happens fast it must be accompanied by a heat release to the environment which is much larger on the average than $k_B T \log 2$. While these ideas may not carry over exactly, optimization and trade-offs of this kind have recently been actively investigated in qubit initialization and reset protocols *e.g.*[18].

Fourth project, on a longer-time horizon, is to analyze quantum thermal engines, which are possible practical applications of the technologies similar to quantum computational devices, and often working in parameter ranges (strong system-bath coupling, etc) that could be called "imperfect". A substantial literature, reviewed in[19], can be summarized to say that quantum thermal machines exist, both theoretically and experimentally, but typically work less well than their classical analogues. On the other hand, it is well known in stochastic thermodynamics that a heat flow can produce information, and, inversely, that information can drive a Maxwell demon[20]. Work can therefore be traded to other resources, and a quantum thermal machine can produce an intrinsically quantum resource, *e.g.* a stationary non-equilibrium heat flow can (in theory) produce entangled states[21]. Even though efficiency is (so far) low, this might in the future be a way to produce entangled states in large quantities.

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[15] T Monnai D Andrieux P Gaspard and Tasaki. "Fluctuation theorem for currents in open quantum systems". In: *New Journal of Physics* 11.10 (Oct. 2009), pp. 109802–109802.

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[17] Erik Aurell et al. "Refined Second Law of Thermodynamics for fast random processes". In: *J. Stat. Phys.* 147 (2012), pp. 487–505.

[18] Jani Tuorila et al. "System-environment correlations in qubit initialization and control". In: *Phys. Rev. Research* 1 (1 Aug. 2019), p. 013004.

[19] Ronnie Kosloff and Amikam Levy. "Quantum Heat Engines and Refrigerators: Continuous Devices". In: *Annual Review of Physical Chemistry* 65.1 (2014), pp. 365–393; Sai Vinjanampathy and Janet Anders. "Quantum thermodynamics". In: *Contemporary Physics* 57.4 (2016), pp. 545–579.

[20] Dibyendu Mandal and Christopher Jarzynski. "Work and information processing in a solvable model of Maxwell's demon". In: *Proceedings of the National Academy of Sciences* 109.29 (2012), pp. 11641–11645.

[21] Jonatan Bohr Brask et al. "Autonomous quantum thermal machine for generating steady-state entanglement". In: *New Journal of Physics* 17.11 (Nov. 2015), p. 113029.