

Extended Abstract for QIP talk:

Error bounds on simulated dynamics of a quantum system coupled to a bosonic environment

Idealized quantum systems may be considered closed, undergoing textbook unitary evolution. In any realistic experimental setup however a quantum system is open, that is, it suffers interactions with an environment composed of those degrees of freedom that are not under the control of the experimenter. Hence the numerical and analytical description of the dynamics of a quantum system interaction with its environment is of fundamental importance in quantum physics. The precise nature and composition of the system-environment interaction is generally not known. For an extremely wide range of systems encountered in physics, chemistry, and biology, it is common to model the environment as a continuum of harmonic oscillators, which interact linearly with the operators of the system. This results in the paradigmatic spin-boson model that captures well many aspects of the system-environment interaction [1]:

$$\hat{H} = \hat{H}_s \otimes \mathbb{1}_B + \mathbb{1}_s \otimes \int d\mathbf{k} g(\mathbf{k}) a_{\mathbf{k}}^\dagger a_{\mathbf{k}} + \mathbb{1}_s \otimes \hat{h} \int d\mathbf{k} f(\mathbf{k}) (a_{\mathbf{k}}^\dagger + a_{\mathbf{k}}). \quad (1)$$

The spin-boson model is exactly solvable only in the rarest of special cases and one is therefore impelled to employ a variety of approximations and numerical descriptions in order to obtain the reduced dynamics of the quantum system in question. Notable examples include those cases in which the environment possesses a correlation time that is much shorter than the system dynamics and the system-environment interaction is weak. Under these assumptions it is then well-justified and customary to resort to the so-called Markov approximation which permits the derivation of linear differential equations, the Lindblad equation, for the quantum system alone [2]. However, settings of considerable practical importance may violate either or both of these assumptions and require a more sophisticated treatment. We give two examples:

1) The recently emerging interest in quantum effects in biological systems provides a case in point [3]. For instance, in typical pigment-protein complexes the dynamical timescales of the vibrational environment can be comparable or even slower than the quantum mechanical excitation energy transfer dynamics. Moreover, in the limit of slow bath dynamics, perturbative treatments of the system-environment coupling cannot be used even if the system-bath coupling is intrinsically weak. In consequence, steps have been taken towards the development of non-perturbative and non-Markovian approaches for the description of the quantum system-environment interaction (see [3, 4] for overviews of recent developments)

2) Models for quantum gravity predict decoherence beyond that of the predictions of quantum mechanics. However, any deviation from the expected behaviour will be small and needs to be proven not to result from an inaccurate simulation of the system-environment interaction. Thus methods that provide rigorous error bounds of the system-environment interaction is of high interest also in fundamental experimental efforts that aim at discovering effects of decoherence beyond the realm of quantum mechanics.

However, generally these approaches have in common that they exploit approximations that are not well controlled in the sense that no rigorous error bounds on the simulation results are available. In this sense these methods are not certified. The time evolving density with orthogonal polynomials algorithm (TEDOPA) approach to the spin-boson model presents a notable exception. It makes use of an exact transformation of the standard representation of the spin-boson model onto a spin interacting with a semi-infinite nearest neighbour coupled chain [5–9] of the form $\hat{H} = \hat{H}_S \otimes \mathbb{1}_B + \hat{h} \otimes \hat{x}_0 + \mathbb{1}_S \otimes \hat{H}_B$ where H_B is infinite dimensional and quadratic in position and momentum variables: $\hat{H}_B = \frac{1}{2} \sum_{i,j=0}^{\infty} (\hat{x}_i X_{i,j} \hat{x}_j + \hat{p}_i P_{i,j} \hat{p}_j)$. This form of the Hamiltonian is particularly amenable to time-adaptive density matrix renormalisation group (t-DMRG) simulations. This approach has been used with success in the simulation of a number of highly non-Markovian system-environment interactions [7, 10, 11]. While the errors that accumulate in the t-DMRG simulation can be bounded rigorously, nevertheless, the numerical TEDOPA simulation employs two as yet uncertified assumptions: (i) the semi-infinite chain needs to be truncated to a finite length and (ii) the local dimension associated with each harmonic oscillator of the chain needs to be truncated to a finite dimensional Hilbert space. Often, it is numerically intractable to estimate the errors that are being introduced in this manner by increasing the chain length and Hilbert space cut-off until results appear to converge. Thus a rigorous approach is desirable. In our work, we employ Lieb-Robinson techniques to close this gap by deriving bounds for the errors arising from approximations (i) and (ii). As the errors arising in each step of the t-DMRG simulation can also be bounded we arrive at a method that possesses rigorous bounds on the results that the simulation of observables obtains.

First we explain our bound for the approximation i). We are interested in bounding the quantity

$$\Delta(t, L) = \left| \text{tr}[\hat{O} e^{-i\hat{H}t} \hat{\rho}_0 e^{i\hat{H}t}] - \text{tr}[\hat{O} e^{-i\hat{H}_L t} \hat{\rho}_0 e^{i\hat{H}_L t}] \right|, \quad (2)$$

i.e., the error introduced when, instead of simulating the full Hamiltonian, simulating the time evolution of system observables \hat{O} with the truncated Hamiltonian $\hat{H}_L = \hat{H}_S \otimes \mathbb{1}_B + \hat{h} \otimes \hat{x}_0 + \mathbb{1}_S \otimes \hat{H}_B^L$, $\hat{H}_B^L = \frac{1}{2} \sum_{i,j=0}^{L-1} (\hat{x}_i X_{i,j} \hat{x}_j + \hat{p}_i P_{i,j} \hat{p}_j)$. Let c such that $\|XP\|^{1/2} \leq c$. We derive the bound

$$\Delta^2(t, L) \leq C \frac{(ct)^{L+2} e^{ct}}{(L+2)!} (\|\gamma_0\|^{1/2} + \|\hat{h}\|t), \quad (3)$$

where $C = 16^2 \|\hat{O}\|^2 \frac{\|\hat{h}\|}{c} \max\left\{ \frac{\|X\|\|P\|}{c^2}, \frac{\|X\|}{c}, \frac{\|P\|}{c} \right\}$, and $\gamma_0 = \begin{pmatrix} \gamma_{xx} & \gamma_{xp} \\ \gamma_{px} & \gamma_{pp} \end{pmatrix}$, $[\gamma_{ab}]_{i,j} = \text{tr}[\hat{a}_i \hat{b}_j \hat{\rho}_0]$, collects the two-point bath correlations in the initial state. If $P = \mathbb{1}$, we may replace L by $2(L-1)$ in the above bound. We derive more general versions of this result in the paper.

We now consider the error introduced when the local Hilbert space dimensions of the bath are truncated, i.e. the error associated with ii). To this end, we define the projector $\mathbb{1}_m = \mathbb{1}_{m_0} \otimes \cdots \otimes \mathbb{1}_{m_{L-1}}$, where $\mathbb{1}_{m_i}$ acts on the i 'th site of the bath and truncates the local Hilbert space according to $\mathbb{1}_m = \sum_{n=0}^m |n\rangle\langle n|$. For bounded observables acting on the system \hat{O} , $\|\hat{O}\| < \infty$, we consider

$$\Delta_m(t) = \left| \text{tr}[\hat{O} e^{-it\hat{H}} \hat{\rho}_0 e^{it\hat{H}}] - \text{tr}[\hat{O} e^{-it\hat{H}_m} \hat{\rho}_0 e^{it\hat{H}_m}] \right|, \quad (4)$$

i.e., the error introduced by evolving the system according to $\hat{H}_m = \mathbb{1}_m \hat{H}_L \mathbb{1}_m$. Thus, with the notation $\hat{x}_i^m = \mathbb{1}_m \hat{x}_i \mathbb{1}_m$ and $\hat{p}_i^m = \mathbb{1}_m \hat{p}_i \mathbb{1}_m$, the truncated Hamiltonian reads $\hat{H}_m = \hat{H}_S + \hat{H}_B^m + \hat{h} \otimes \hat{x}_0^m$, where $\hat{H}_B^m = \frac{1}{2} \sum_{i,j=0}^{L-1} [X_{i,j} \mathbb{1}_m \hat{x}_i \hat{x}_j \mathbb{1}_m + P_{i,j} \mathbb{1}_m \hat{p}_i \hat{p}_j \mathbb{1}_m]$, we show that

$$\frac{\Delta_m^2(t)}{4\|\hat{O}\|^2} \leq \text{tr}[(\mathbb{1} - \mathbb{1}_m)\hat{\rho}_0] + 2 \int_0^t dx \sqrt{\epsilon_m(x)} \quad (5)$$

and $\epsilon_m(x)$ is given in the accompanying paper. Crucially, under the assumption that the system Hilbert space is finite dimensional, this error may be computed numerically as it involves *only* observables acting on the truncated Hilbert space and which are of a form amenable to t-DMRG simulations. For all finite times, $\lim_{\{m_i\} \rightarrow \infty} \Delta_m = 0$ and for all finite m , and L , Δ_m is bounded from above by a linearly increasing function in t . $\text{tr}[(\mathbb{1} - \mathbb{1}_m)\hat{\rho}_0]$ is zero for any initial finitely many particle bath state when m is chosen appropriately. Such states include the vacuum state which is also the zero Kelvin thermal state. For higher temperature thermal states of the bath, it is expected to decay rapidly when increasing all the m_i 's. The total error induced on the expectation value of \hat{O} due to (i) and (ii) is bounded by the sum of the two individual error bounds: $\Delta(t, L) + \Delta_m(t)$. This bounds the error of approximating an infinite dimensional bath of bosons by a length L 1-D spin chain with nearest neighbour interactions. If in addition we assume the system to be a spin system, then the Hamiltonian is in the class which [12] shows can be simulated with polynomial resources in L and error ϵ , and exponential in $|t|$.

This extends significantly existing recent results in the literature that apply to the finite dimensional setting of spin systems [12] and therefore allows the fully certified treatment of the system-environment interaction for both, harmonic oscillator as well as spin environments. The bound we develop for approximation (i) is closely related to the Lieb-Robinson bound, which bounds the time evolution of the commutator of local observables [13] and physically means that there is a finite speed at which information propagates through the lattice. Our work also constitutes a significant step forward in the class of Hamiltonians which are proven to admit locality bounds. Due to the unboundedness of the Hamiltonian, these bounds are very difficult to prove and very little is known. Prior to this work, in the unbounded setting, harmonic systems and a class of anharmonic perturbations of them [14–16] and more recently Hamiltonians linear in spin operators and quadratic in the boson position/momentum operators [17] were known to admit the bound.

In summary, we provide the first bounds which allow one to calculate error bars for the approximations made in numerically challenging simulations of spins interacting with a continuum of bosons. Without these results, doing numerics for such systems (which are of high practical importance, see 1), 2) above) is analogous to doing an experiment in which one collects experimental data *without* the possibility to put error bars to the data set.

[1] A.J. Leggett, S. Chakravarty, A.T. Dorsey, M.P.A. Fisher, A. Garg, and W. Zwerger, Rev. Mod. Phys. **59**, 1 (1987).

[2] A. Rivas and S.F. Huelga, *Open Quantum Systems: An Introduction*. Springer Briefs in Physics, Springer Verlag 2012.

- [3] S.F. Huelga and M.B. Plenio, *Contemp. Phys.* **54**, 181 (2013).
- [4] L.A. Pachon and P. Brumer, *Phys. Chem. Chem. Phys.* **14**, 10094 (2012).
- [5] R. Burkey, C. Cantrell, *J. Opt. Soc. Am. B.* **1**, 169 (1984)
- [6] R. Bulla, H. Lee, H. Tong, M. Vojta, *Phys. Rev. B.* **71**, 045122 (2005)
- [7] J. Prior, A.W. Chin, F.S. Huelga, M.B. Plenio, **105**, *Phys. Rev. Lett.* **105**, 050404 (2010)
- [8] A. Chin, A. Rivas, S.F. Huelga, M.B. Plenio, *J. Math. Phys.* **51**, 092109 (2010)
- [9] R. Martinazzo, B. Vacchini, K.H. Hughes, I. Burghardt, *J. Chem. Phys.* **134**, 011101 (2011)
- [10] J. Prior, I. de Vega, A. Chin, S.F. Huelga, M.B. Plenio, *Phys. Rev. A.* **87**, 013428 (2013)
- [11] A.W. Chin, J. Prior, R. Rosenbach, F. Caycedo-Soler, S.F. Huelga, M.B. Plenio, *Nat. Phys.* **9**, 113 (2013)
- [12] T. Osborne, *Phys. Rev. Lett.* **97**, 157202 (2006)
- [13] B. Nachtergaele, R. Sims, *Contemporary Mathematics*, A.M.S. **529**, 141 (2010)
- [14] M. Cramer, A. Serafini and J. Eisert, *Quantum information and many body quantum systems*, Eds. M. Ericsson, S. Montangero, Pisa: Edizioni della Normale, pp 51-72, 2008 (Publications of the Scuola Normale Superiore. CRM Series, 8)
- [15] B. Nachtergaele, H. Raz, B. Schlein, R. Sims *Commun. Math. Phys.* **286**, 1073 (2008)
- [16] U. Islambekov, R. Sims, G. Teschl, *J. Stat. Phys.* **3**, 440 (2012)
- [17] J. Juenemann, A. Cadarso, D. Perez-Garcia, A. Bermudez, J.J. Garcia-Ripoll, *Phys. Rev. Lett.* **111**, 230404 (2013)