nature portfolio

Peer Review File

Quantum Simulation of Spin-Boson Models with Structured Bath

Corresponding Author: Professor Jungsang Kim

This file contains all reviewer reports in order by version, followed by all author rebuttals in order by version.

Version 0:

Reviewer comments:

Reviewer #1

(Remarks to the Author)
The manuscript presents a very flexible implementation of a spin-boson model coupled to structured environments. Through the astute addition of randomized control parameters, the authors effectively implement a 'stochastic unraveling' of the Lindblad dynamics. This approach is benchmarked for quantum simulations of vibrationally assisted energy transfer and the coupling to sub- and super-ohmic baths.

I think this platform is likely to influence the development of analog quantum simulations of chemical processes, including energy or electron transfer in the presence of coupling to structured environments. This is why I think this work could be publishable in Nature Communications, even though it does not report an advance beyond the capabilities of classical computers. In particular, the simulation of the approximate generation of sub- to super-ohmic spectral baths opens the possibility to explore non-Markovian quantum dynamics with unprecedented control.

However, since this work has to be considered a proof of concept, a discussion of potential limitations of this platform (number of modes, variability of coupling strengths, scaling of the number of experimental runs for convergent results) should be elaborated in the Discussions section, which currently focuses on potential applications solely. For instance, it would be important to know how, or to what extent the number of phonon modes may be increased. Simply increasing the number of ions will surely lead to more closely spaced eigenmodes and hence lead to undesirable crosstalk between modes? For the benefit of the reader, this should be explained carefully.

- Fig. 4: why is there a different number of trials in panels b)-d) ?

- Ref. 34 is by now published in Science Advances.

- Following Eq. 1, " the spin is in the $|0\rangle$ state (“donor” state)", but the $|1\rangle$ state is never introduced as the acceptor is never introduced. The nomenclature also does not make much sense in the context of this paper, where several 'abstract' models are introduced.

Reviewer #2

(Remarks to the Author)
The manuscript by Ke Sun et al. describes a method for producing open system dynamics in a trapped-ion quantum simulator. As described in the introduction, open quantum system dynamics are important to consider for understanding quantum phenomena in chemistry, optics, biology, and information science where energy can flow between systems. At a high level, this manuscript describes an additional tool the authors have developed for the trapped ion quantum simulator platform. The ability to apply custom (or at least tunable) dissipative bath profiles to quantum spin model simulations with tens or hundreds of qubits could advance near-term quantum simulators toward the realm of quantum advantage over

classical approaches. This manuscript describes an initial step toward that goal by experimentally demonstrating a well-calibrated, programmable dephasing mechanism in a short ion chain.

This scheme implements a spin-boson model by encoding a spin degree of freedom in a trapped-ion's internal electronic state and a quantum harmonic oscillator bath in the ion chain's motional (bosonic) modes. Spin-dependent kick operations, similar to the laser-driven operations used to implement the famous MøImer–Sørensen entangling gate, drive interactions between the ion's spin and the ion chain's motional modes. In Section 2 "Dephased Spin-Oscillator Model" the authors provide a good description of regimes where their simulation approach is valid. The discussion is fairly long and dense, but this is acceptable since there are many important Hamiltonian parameters and relationships to define here.

Figure 2a demonstrates how the initial temperature of the ion chain impacts information retention in the spin. This matches an intuitive picture of the spin-boson model: a hot bath should dephase a spin faster than a cold bath. The data presented in Figure 2 showcases the authors' ability to program motional mode temperatures and effective Hamiltonian parameters.

Figure 3 shows how two different dissipative bath structures, generated by driving two and three motional modes respectively, impact the spin dynamics. Spin evolutions in Figure 3c match theory curves well. This indicates that the "engineered noise" is not substantially degraded by unintentional experimental noise. The authors either minimize sources of baseline noise in their experiment well, characterize the baseline noise in their experiment very well, or likely both.

Figures 4 and 5 further demonstrate the tunability of this method. I found Figure 4 to be the most impressive data of this manuscript. Here the authors simulate a "textbook" version of the spin-boson model in order to demonstrate clean examples of Ohmic dissipation (4b, 4c, and 4d).

In summary, this manuscript describes a method for simulating open system dynamics in a small but well-controlled trapped-ion quantum simulator. The paper and supplement contain extensive theoretical and experimental background. Several of the important techniques used in the experiment are inspired by past work, and these are sufficiently cited (for instance References 15 suggests coupling a trapped-ion spin to multiple motional modes for a structured bath, and Reference 38 suggests the trick of averaging over noisy simulations to achieve Markovian dynamics). This method, combined with additional controls, observables, and larger system sizes, could contribute to useful quantum simulations beyond classical capabilities.

I request that Ke Sun et al. consider several questions and comments below. Once these are addressed, I will I recommend publication of the manuscript in Nature Communications.

Questions and Comments for the Authors:

Near the end of the introduction the authors state that they use their programmable dephasing control to study the dynamics of "classic spin-boson models". I strongly suggest the authors reconsider the word "classic" here. During my first read of the Introduction I mistakenly read this as "classical spin-boson models", which led to great confusion. Nature Communications has a broad audience and I fear readers could make similar mistakes. I suggest "standard", "typical", or "conventional" instead of "classic".

Typos in section "Experimental Implementation", second paragraph: I believe "time evolution operators" should be plural. The sentence is also missing an article "the": "…in the Hamiltonian in the interaction picture…"

Near the end of "Dephased Spin-Oscillator Model," consider mentioning shelving or optical-metastable-ground state (omg)-type encoding as another method for damping with sympathetic cooling.

I find the rescaled times in Figures 3c and 5 somewhat confusing. I understand this connects the results with potential applications, and that may help molecular energy transfer researchers grasp the data. But as a researcher unfamiliar with that particular application, I felt the parameter mapping to be somewhat arbitrary. It may help if the x-axis labels were changed to "effective time" or "molecular time" or similar? Apologies that I likely failed to understand something here.

In the Figure 1 caption and Section I.A of the supplement, the authors discuss driving only the center ion of an odd-numbered ion chain to avoid coupling to unwanted motional modes. The SDK laser tones (see Figure 3b) only drive the symmetric motional modes (modes 3, 5, and 7). These clever experimental design choices likely contribute to the successful experiments in this manuscript. However, I am concerned about this method's scalability. Could you please describe how the number of useful modes scales as the number of ions increases? Would poor scaling impact this method's usefulness with longer chains? I haven't done any calculations on this, but I have a hunch that the number of symmetric modes grows more slowly than the number of ions. I.e., adding 2 ions adds only 1 useful mode and so on.

Reviewer #3

(Remarks to the Author)
The authors report an analog quantum simulation of spin-boson models driven by a tuneable bath. The paper is very timely, coming at a time of high interest in analog quantum simulation and of experimental techniques that are able to achieve interesting results. The ion trap platform the authors use is particularly

promising due it its low characteristic noise, as evidenced in the high-quality results obtained.

In my view, this is one of the most impressive results in bath engineering for analog simulation. In particular, the ability to combine as many as three modes with different widths is an impressive achievement.

The authors also correctly identify, in the Discussion section, broad avenues for future work and broader applicability of their method.

The work reported in the manuscript is of high quality and the paper is well written, so I recommend it for publication in Nature Communications.

I have had the benefit of reviewing this manuscript when it was submitted to a different journal, and the authors have implemented my suggestions very well, so that, as a result, I only have one remaining remark.

On p 9 and in Fig 4, the authors claim to implement simulations of Leggett models with different s (giving Ohmic, sub-ohmic, or super-ohmic spectral densities). In my view, the experimental evidence is consistent with the simulation goals, but it is insufficient to make claims that the simulation is able to distinguish sub/super/Ohmic spectral densities. The reason for saying this is that the system resonance is very narrow, so the system can only respond to the value of the spectral density at resonance, and not to the shape of the spectral density (which is controlled by s). The authors get it right on p 9 when they attribute differences "owing to the different levels of spectral density $J(\omega = \Delta)$ near resonance", but then make the mistake of saying that "The observed behavior qualitatively
agrees with the predictions of the Leggett model: for super-Ohmic case, coherence
is maintained due to low spectral density near resonance, while for sub-Ohmic case,
large spectral density induces strong damping to the point where the system is localized."
It is *not* a feature of the Leggett model that, for example, the super-ohmic case has "low spectral density near resonance". For any value of s, the value of the spectral density at resonance is independent of s: it's possible to have both strong and weak damping at resonance no matter what the s is. A system needs to have multiple frequencies for a distinction between spectral densities to make sense. So my advice to the authors is to not talk about different s at all, and just present their results as a series of spectral densities they simulated, whose effect on the single-frequency system can be explained by the strength of the spectral density at resonance.

Version 1:

Reviewer comments:

Reviewer #1

(Remarks to the Author)
The authors have addressed the (minor) concerns of the first round of reviews, and so I am happy to recommend the publication of this nice work.

Reviewer #2

(Remarks to the Author)
The authors sufficiently addressed all my points. I recommend the revised manuscript for publication in Nature Communications.

Reviewer #3

(Remarks to the Author)
I'm satisfied with the authors' response. Although I did suggest they remove discussions of super/sub/Ohmic spectral densities, which cannot be resolved by their experiment, their text is not incorrect, and it can be published if they insist.

I would point out one thing I might have missed last time. On page 9, the description "The spin dynamics are expected to exhibit a
phase transition from coherent oscillations to incoherent decay or localization as s is decreased or the amplitude A is increased" is incorrect on two counts. First, this is not a phase transition because it is smooth and it occurs even in single donor-acceptor pairs and does not require the thermodynamic limit. Second, there would be no such transition with respect to s in the present case, where there is a narrow resonance and the rate of damping depends only on A. The general statement referred to is true in more realistic models of energy transfer with broad densities of states.

I do not need to see the manuscript again.

We would like to thank the reviewers for their thoughtful comments, feedback and questions, which we find to be pertinent and helpful in improving the presentation of our work to the readers. Here, we provide our responses to the reviewers' comments, and the corresponding changes that were made in the revised manuscript.

1 Response to Reviewer 1

General Overview:

The manuscript presents a very flexible implementation of a spin-boson model coupled to structured environments. Through the astute addition of randomized control parameters, the authors effectively implement a 'stochastic unraveling' of the Lindblad dynamics. This approach is benchmarked for quantum simulations of vibrationally assisted energy transfer and the coupling to sub- and super-ohmic baths.

I think this platform is likely to influence the development of analog quantum simulations of chemical processes, including energy or electron transfer in the presence of coupling to structured environments. This is why I think this work could be publishable in Nature Communications, even though it does not report an advance beyond the capabilities of classical computers. In particular, the simulation of the approximate generation of sub- to super-ohmic spectral baths opens the possibility to explore non-Markovian quantum dynamics with unprecedented control.

Our Response: We appreciate Reviewer 1's thoughtful and encouraging feedback. We are delighted that the reviewer recognize the flexibility of our approach and its potential impact on analog quantum simulations of chemical processes. Our goal was to provide a robust framework for studying spin-boson interactions in structured environments, and we appreciate the insights into its broader implications, particularly for energy and electron transfer dynamics.

We also value the reviewer's perspective on the relevance of our work despite its accessibility to classical computation. We sincerely appreciate the support and con-

structive evaluation, and we hope that our work contributes meaningfully to the field.

However, since this work has to be considered a proof of concept, a discussion of potential limitations of this platform (number of modes, variability of coupling strengths, scaling of the number of experimental runs for convergent results) should be elaborated in the Discussions section, which currently focuses on potential applications solely. For instance, it would be important to know how, or to what extent the number of phonon modes may be increased. Simply increasing the number of ions will surely lead to more closely spaced eigenmodes and hence lead to undesirable crosstalk between modes? For the benefit of the reader, this should be explained carefully.

Our Response: We appreciate the reviewer for the suggestion. Indeed, there remain challenges and open questions for this type of spin-boson systems to scale. We added a paragraph to the "Discussion and Outlook" section containing the following points: (1) how the number of modes and coupling strengths scale as a function of the ion chain length, (2) the transverse mode spacing and ways to manage them, and (3) challenges in characterizing the boson modes. We also added Sec. VII in the Supplementary Material to further discuss how the cross-mode coupling can be reduced.

We address specific comments below.

1. *Fig. 4: why is there a different number of trials in panels b)-d) ?*

Our response: In Fig. 4(b), the ion spin decays more rapidly compared to the other two scenarios, leading to a stationary state around $P(|D\rangle) = 0.5$, which has a larger standard deviation due to the binomial distribution. Increasing the number of trials can help reduce the overall deviation and improve precision. We include the explanation in the figure caption.

2. *Ref. 34 is by now published in Science Advances.*

Our response: We now cite the reference in the main text describing the use of sympathetic cooling to simulate dissipation.

3. *Following Eq. 1, " the spin is in the $|0\rangle$ state ("donor" state)", but the $|1\rangle$ state is never introduced as the acceptor is never introduced. The nomenclature also does not make much sense in the context of this paper, where several 'abstract' models are introduced.*

Our response: We appreciate the reviewer for pointing this out. We introduced both "donor" and "acceptor" states as well as clarified that these terms are used in the context of energy transfer model.

2 Response to Reviewer 2

General Overview:

The manuscript by Ke Sun et al. describes a method for producing open system dynamics in a trapped-ion quantum simulator. As described in the introduction, open quantum system dynamics are important to consider for understanding quantum phenomena in chemistry, optics, biology, and information science where energy can flow between systems. At a high level, this manuscript describes an additional tool the authors have developed for the trapped ion quantum simulator platform. The ability to apply custom (or at least tunable) dissipative bath profiles to quantum spin model simulations with tens or hundreds of qubits could advance near-term quantum simulators toward the realm of quantum advantage over classical approaches. This manuscript describes an initial step toward that goal by experimentally demonstrating a well-calibrated, programmable dephasing mechanism in a short ion chain.

...

In summary, this manuscript describes a method for simulating open system dynamics in a small but well-controlled trapped-ion quantum simulator. The paper and supplement contain extensive theoretical and experimental background. Several of the important techniques used in the experiment are inspired by past work, and these are sufficiently cited (for instance References 15 suggests coupling a trapped-ion spin to multiple motional modes for a structured bath, and Reference 38 suggests the trick of averaging over noisy simulations to achieve Markovian dynamics). This method,

combined with additional controls, observables, and larger system sizes, could contribute to useful quantum simulations beyond classical capabilities.

Our Response: We appreciate Reviewer 2's recognition of our work as an important step toward simulating open quantum system dynamics using a trapped-ion quantum simulator. Our goal was to develop a versatile approach for engineering tunable dissipative bath profiles, and we are pleased that the reviewer sees its potential in advancing near-term quantum simulators toward demonstrating quantum advantage.

We also appreciate the acknowledgment of the theoretical and experimental background provided in the manuscript and supplement, as well as the proper citation of relevant prior work. While our current implementation focuses on a small, well-controlled system, we are excited about the possibility of scaling this method to larger ion chains and incorporating additional controls and observables to further explore complex quantum dynamics.

We address specific comments below.

1. *Near the end of the introduction the authors state that they use their programmable dephasing control to study the dynamics of "classic spin-boson models". I strongly suggest the authors reconsider the word "classic" here. During my first read of the Introduction I mistakenly read this as "classical spin-boson models", which led to great confusion. Nature Communications has a broad audience and I fear readers could make similar mistakes. I suggest "standard", "typical", or "conventional" instead of "classic".*

Our response: We fixed "classic" to "typical" as suggested.

2. *Typos in section "Experimental Implementation", second paragraph: I believe "time evolution operators" should be plural. The sentence is also missing an article "the": "... in the Hamiltonian in the interaction picture..."*

Our response: We fixed the typos as suggested.

3. *Near the end of "Dephased Spin-Oscillator Model," consider mentioning shelving or optical-metastable-ground state (omg)-type encoding as another method for damping with sympathetic cooling.*

Our response: We mentioned omg encoding as a potential method for simulating damped oscillators and cited [D.T.C. Allcock et al., Appl. Phys. Lett. 119, 214002 (2021)].

4. *I find the rescaled times in Figures 3c and 5 somewhat confusing. I understand this connects the results with potential applications, and that may help molecular energy transfer researchers grasp the data. But as a researcher unfamiliar with that particular application, I felt the parameter mapping to be somewhat arbitrary. It may help if the x-axis labels were changed to "effective time" or "molecular time" or similar? Apologies that I likely failed to understand something here.*

Our response: We revised the captions of the Figs. 3 and 5 to explain the x-axis.

5. *In the Figure 1 caption and Section I.A of the supplement, the authors discuss driving only the center ion of an odd-numbered ion chain to avoid coupling to unwanted motional modes. The SDK laser tones (see Figure 3b) only drive the symmetric motional modes (modes 3, 5, and 7). These clever experimental design choices likely contribute to the successful experiments in this manuscript. However, I am concerned about this method's scalability. Could you please describe how the number of useful modes scales as the number of ions increases? Would poor scaling impact this method's usefulness with longer chains? I haven't done any calculations on this, but I have a hunch that the number of symmetric modes grows more slowly than the number of ions. I.e., adding 2 ions adds only 1 useful mode and so on.*

Our response: We appreciate the reviewer for bringing up this point. Our choice of symmetric modes in this work was intentional, as it helps minimize cross-mode coupling. However, there are alternative methods to reduce cross-mode coupling (see the newly added paragraph in the end of "Discussion and Outlook" section in response to Reviewer 1). Using only symmetric modes is not necessary if the cross-mode coupling can be managed, allowing us to leverage all available motional modes coupled to all qubits in the ion chain.

Additionally, since ions move in three directions, the total number of motional modes is three times the number of ions. Our current experimental setup is designed to couple only to one transverse direction, limiting the usable number of motional modes to be equal to the number of ions, but it is straightforward to work with both transverse directions.

3 Response to Reviewer 3

General Overview:

The authors report an analog quantum simulation of spin-boson models driven by a tuneable bath. The paper is very timely, coming at a time of high interest in analog quantum simulation and of experimental techniques that are able to achieve interesting results. The ion trap platform the authors use is particularly promising due it its low characteristic noise, as evidenced in the high-quality results obtained.

In my view, this is one of the most impressive results in bath engineering for analog simulation. In particular, the ability to combine as many as three modes with different widths is an impressive achievement.

The authors also correctly identify, in the Discussion section, broad avenues for future work and broader applicability of their method.

The work reported in the manuscript is of high quality and the paper is well written, so I recommend it for publication in Nature Communications.

Our Response: We thank the reviewer for the positive and encouraging feedback. We are delighted that the reviewer find our work timely and recognize the potential of the trapped-ion platform for analog quantum simulation. The appreciation of our bath engineering approach, particularly the ability to combine multiple motional modes with different widths, is truly gratifying.

We also appreciate the acknowledgment of the broader applicability of our method and the future directions outlined in the Discussion section. Our goal was to develop a flexible and high-precision approach to simulating spin-boson interactions, and we

are pleased that the reviewer see its potential impact.

*On p 9 and in Fig 4, the authors claim to implement simulations of Leggett models with different s (giving Ohmic, sub-ohmic, or super-ohmic spectral densities). In my view, the experimental evidence is consistent with the simulation goals, but it is insufficient to make claims that the simulation is able to distinguish sub/super/Ohmic spectral densities. The reason for saying this is that the system resonance is very narrow, so the system can only respond to the value of the spectral density at resonance, and not to the shape of the spectral density (which is controlled by s). The authors get it right on p 9 when they attribute differences "owing to the different levels of spectral density $J(\omega = \Delta)$ near resonance", but then make the mistake of saying that "The observed behavior qualitatively agrees with the predictions of the Leggett model: for super-Ohmic case, coherence is maintained due to low spectral density near resonance, while for sub-Ohmic case, large spectral density induces strong damping to the point where the system is localized." It is *not* a feature of the Leggett model that, for example, the super-ohmic case has "low spectral density near resonance". For any value of s, the value of the spectral density at resonance is independent of s: it's possible to have both strong and weak damping at resonance no matter what the s is. A system needs to have multiple frequencies for a distinction between spectral densities to make sense. So my advice to the authors is to not talk about different s at all, and just present their results as a series of spectral densities they simulated, whose effect on the single-frequency system can be explained by the strength of the spectral density at resonance.*

Our Response: While our intention was to compare the sub-Ohmic, Ohmic, and super-Ohmic baths with fixed A and ω_c values, we agree that the sentence pointed out by the reviewer can be misleading. We removed the sentence and instead guide the readers to Sec. VI of the Supplemental Material, where we compare the baths with fixed $J(\omega = \Delta)$ value.