Summary -

In SciPost manuscript number 202408, with the title "*Dynamics of systems with varying number of particles: from Liouville equations to general master equations for open systems*", the authors discuss various approaches for treating mostly classical systems that have varying numbers of particles, culminating in a formalism that they claim is novel and provides a unified framework capable of opening up new research pathways. It is undeniable that systems with varying particle numbers are crucial in a wide range of fields, from physics to chemistry to population dynamics. I agree, therefore, that a review of the various approaches as well as a formalism that unifies them would be valuable, at least as a teaching tool if nothing else. However, I find that the way these methods are discussed and the presentation of the unifying approach to be flawed. Consequently, I would not approve the manuscript for publication without significant review.

Major Comments

- I find the overall purpose and message of the paper to not be clear. When I started reading it, I got the impression that the authors were going to not only discuss previous attempts at treating systems with varying numbers of particles, but also introduce an essentially new, comprehensive framework that one can apply to a wider variety of systems, with specific illustrating examples and perhaps even with connections to other fields (e.g. "social agent-based dynamics" in the abstract). This is essentially what is promised in the abstract.

  But when I actually read the paper, I found it to be more a collection of the authors' various works from the past few years with the observation that they often derive master equations with similar forms between the various methods. I did not see any results presented for a specific example model and it was not clear to me how the unified framework can actually be used for anything truly novel, or how it can concreteley be used to go beyond current approaches. I did not really see a connection to other fields; the authors say that there are connections to the spread of diseases, innovations, etc in Sec. VI, but there is no mention of how one might actually go about this. I think the authors should stress that this is a review paper rather than advertising the "unifying master equation" as the main result. I actually found the reviews they wrote of their methods to be comprehensive and a good insight into their work.

- I think that a few figures have appeared in the authors' previously published works. Something very similar to Fig. 3a, for example, can be found in Chapter 21 of Biomolecular Simulations (2013), Volume 92, while Fig. 4 appears in Fig. 1 of this this arxiv preprint from this year, and something very similar to Fig. 2 appears in Fig. 1 of J. Math. Phys. 61, 083102 (2020) and Fig 1 of Adv. Theory Simul. 2019, 2, 1900014. I think that the figure captions should at least say when a figure has been adapted from previous work. More importantly, I found it hard when reading the paper to distinguish between what is new work and what is a discussion of previously published work. This extends to the figures when they are just presented as they are with no discussion

about where they come from or if indeed they were generated solely for this work. Maybe the editor can provide more guidance on what is appropriate here.

- The authors state clearly in the abstract that they not only discuss approaches for treating systems with varying particle numbers, but also formulate a unifying master equation, essentially promising something new. Furthermore, in Sec. II, they emphasise that the main results are from that section and Sec. V, which discusses connections between the various approaches. But they also acknowledge at the end of Sec. II that very similar master equations have appeared in the literature before, both from their own recent work and also from working dating back to 1962. Eq.(4), for example, appears essentially in Eq. 13 of Ref. 14, with only very minor notation differences. I guess that the authors' argument would be that they formulated Eq. 13 in Ref. 14 specifically as a chemical diffusion master equation, whereas Eq.(4) of this work is more general, but it is not really clear to me what is more general about this formulation? In Eq.(53) where they connect the two approaches, they say that $\mathcal{A}_n f_n \to \mathcal{D}_n f_n$, where $\mathcal{D}_n$ is the standard Brownian diffusion. But in Ref. 14, Eq.(8), they also formulate it for a general Fokker-Planck operator, so I am not sure really what the difference is here?

- I can apply similar critique to Sec. III A, where the authors discuss Liouville-like equations for classical open systems as well as the AdResS method. The section is basically a summary of the authors' recent works, see Refs. 19, 20, and 44, but I am not sure exactly how novel such a discussion is. Specifically, I do not understand why the AdResS part is necessary. The idea is to show that integrating out the reservoir dofs for a classical open system yields an equation that fits the form of Eq.(4), the equation connecting all methods in the paper. Why is it necessary, then, to additionally present their specific algorithm?

- These points aside, I do not totally understand what extra information or numerical pathways the unified framework brings. The authors consistently state throughout the manuscript that their unifying framework can applied to a wide variety of problems and opens up new research pathwasy, but the text does not make it clear to me exactly how. Consider this sentence from Sec. VI :

  "*The material exchange can model reactions, interactions with a reservoir or any other process that changes the number of particles. Analyzing and manipulating these components offer insights into the intricate interplay between system dynamics and its surroundings, shedding light on emergent behaviors and equilibrium states.*"

  What light does their approach shed on emergent behaviors and equilibrium states?

  "*The form of eq. (56) hints at the possibility of performing a two-level coarse-graining of a Hamiltonian system. First, coarse-graining the fast-scales, e.g. the solvent dynamics into a thermostat. Then, a second coarse-graining following section III A to model the material exchange of the subsystem with the environment. Although these two effects produced by different types of reservoir interaction were also captured in the seminal work [49] with equations in the form of eq. (22), the approach here presented is more general and conceptually different.*

Their approach may be more general and a little conceptually different, but this is one of the only instances where they suggest a specific approach motivated by their unified framework, except that it has already been suggested in Ref. 49.

Consider also:

"*This last property is why it is suitable for data-driven methods. To the best of our knowledge, we are not aware of the construction or application of the Koopman operator for particle-based systems with varying copy numbers, such work would precipitate applications on diverse fields and this work provides the cornerstones to construct it.*

How does their work provide the cornerstones to do it? How would they apply the general formalism here to this problem?

I understand that the authors are trying to provide an overview of where a general master equation framework for systems with varying numbers of particles could be used, but as a reader, I remain unconvinced when there are no specifics of how one might translate the work to these fields at all.

- The authors restrict most of their introduction, theory, and discussion to classical open systems, which is understandable given the unique challenges that quantum approaches hold. However, there are some instances where they try to connect their work to open quantum systems, and these statements confuse me a little. In Sec. VI, for example, the authors state that

  "*However, to the best of our knowledge, the Lindblad equation in its most common form employed in the literature cannot describe the exchange of particles in equilibrium between the system and the environment.* "

  If one formulates the Lindblad equation for a system-bath setup in which the bath is explicitly a heat bath, such as in the spin-boson model, then of course the Lindblad operators will describe dissipation via heat exchange. But there is an extensive history of Lindblad-type and other master equations being used for system-reservoir setups in which particles are exchanged. A standard example would be theoretical treatments of charge transport through molecular nanojunctions, in which one applies a voltage bias between two metal electrodes, such that a current flows through a molecule or other quantum system placed in the middle. One can use a variety of approaches for these types of systems, but one of the most prevalent is the master equation method. Here, the changing-particle-number perspective is built directly into the model and appears explicitly in the reduced density matrix of the open quantum system, ρ. In fact, the master equations for these types of systems have pretty much the exact form of Eq. (4) of this work. Note that one can use a Lindblad or master equation in or out of equilibrium; the formalism remains the same.

  The authors even mention these types of approaches in their mentioning of Refs. 14, 23, and 24, where the ideas of the Fock space are applied to classical systems to derive similar equations of motion as in the quantum case. They also reference their own work in Ref. 18, in which they acknowledge that there are quantum master equations where the number of particles is a variable

of the problem. In this reference, they also make the claim that the limiting case of equilibrium has not been applied to quantum master equations, and this seems to be their overall point, but I do not know exactly what they mean. A quantum master equation can be applied both in and out of equilibrium. What exactly do the authors mean here?

Minor Comments

- I was confused about this sentence:

  "*To exemplify the formulation of the CDME for a reaction involving only one chemical species, we focus on a reaction that models social friction in population dynamics (fig. 3b.)*"

  Do the authors really reference population dynamics here? In the caption of Fig.3b, it refers to particle-based reaction-diffusion processes instead.

- The authors should be careful with small typos and inconsistencies in notation. A small but not exhaustive list:

  - In the abstract:

    "*... but enables modeling a much larger range of complex systems*"

    should be

    "*... but enables modeling of a much larger range of complex systems*"

  - In the introduction:

    "*... the equations proposed in Refs.25, 30, 59, 65, 67, ...*

    should be

    "*... the equations proposed in Refs.[25, 30, 59, 65, 67], ...*

    if they want to be consistent with other parts of the text.

  - Sometimes they use different notation for referencing the figures, e.g. Figure 1, Fig.2, fig. 3. This should be consistent throughout.