Comment on: “Fluctuation Theorem for Many-Body Pure Quantum States”

Iyoda et al. present a general argument which is intended to (literal quotation of the first sentence of the abstract) “… prove the second law of thermodynamics and the non-equilibrium fluctuation theorem for pure quantum states” [1]. To exemplarily back up this statement, they perform a numerical analysis of a lattice model of interacting hard-core bosons.

In this comment we point out the following: While the argument is mathematically sound, it can hardly be applied to the physical situations to which fluctuation theorems and/or the second law routinely refer. Its validity is limited to rather extreme time and length scales far away from said physical situations. This is due to Lieb-Robinson speeds being too high, relevant processes lasting too long, and baths being too small in standard setups. A careful analysis of the above numerical example reveals that the results supporting the theorem only occur for a selective choice of the parameters and/or coincide with the short initial period during which the system only negligibly leaves its initial state, i.e., the system practically “does nothing”.

Central to the argument in [1] is a conceptual division of the bath $B$ into a near bath $B_1$ and a far bath $B_2$, in spite of the full physical bath just being one homogeneous system. The considered system is only coupled to an edge of the near bath $B_1$. Now the claims in [1] hold under two conditions: (i) The reduced state of $B_1$ must result as a strictly Gibbsian state for an energy eigenstate on the full bath $B$. (This corresponds to the eigenstate thermalization hypothesis (ETH).) (ii) All considered times must not exceed the minimum time at which energy, information, particles, etc. could possibly cross $B_1$ (Lieb-Robinson time).

Before we embark on a consideration of realistic time and length scales, let us settle the required ratio of sizes of $B_1$ and $B_2$. If $B_1, B_2$ were non-interacting, a mixed microcanonical state from an energy shell of the full bath would result in a canonical state on $B_1$ only if the density of states of $B_2$ was well described by an exponential $e^{\beta E}$ over the full energetic spectrum of $B_1$. This, however, requires that ($B_1$ and $B_2$ are indeed structurally identical systems) $B_2$ must be larger than $B_1$ by at least a factor of ten or so. Thus, even if the ETH nicely applies and the actual interaction between $B_1, B_2$ is negligible (for details cf. [3]), the ratio must be at least, say, 1:10 to get a reduced canonical state on $B_1$. To grasp the gist of the problem of relevant scales, consider standard experiments in the context of the Jarzynski relation (which is a prime example of a fluctuation relation): the unfolding of proteins (cf., e.g., [4]). These experiments are done in aqueous solution. While the (conceptual) Lieb-Robinson speed of water is hard to determine, it must at least exceed the respective speed of sound, ca. 1400 m/s. The time scales on which these experiments are performed are on the order of seconds. Thus, for the argument of Iyoda et al. to hold, the near bath $B_1$ would have to be ca. 1.4 km large. Consequently, the far bath $B_2$ would have to be 14 km large. The vessels in which these experiments are actually performed are, however, on the order of centimeters. Thus, this scheme cannot explain the applicability of a standard fluctuation theorem in a standard setting. Similarly, to explain the validity of the second law according to [1] for a cup of coffee that cools down during, say, ten minutes, one would need ca. 200 km of undisturbed air around the cup as $B_1$, which amounts to a volume of air on the scale of 2000 km as $B_2$. These facts are in sharp contrast to statements like (literal quotation): “Our result reveals a universal scenario that the second law emerges from quantum mechanics, …” and “…, in this Letter we rigorously derive the second law of thermodynamics for isolated quantum system in pure states.” Note that [1] does not offer any discussion of an upper bound to the Lieb-Robinson based on realistic sizes of concrete systems, but exclusively focuses on the hypothetical limit of infinitely large baths.

While the numerics in [1] appear to confirm the impact of the theoretical reasoning on concrete quantum dynamics at first sight, more thorough analysis reveals that this is not the case. To elucidate this, we re-did the numerics in [1] but (i) applied the original parameters to both dynamical quantities considered in [1], (ii) checked the effect of changing one parameter, and (iii) additionally computed a simple observable that indicates how much the system is evolving at all.

The first claim in [1] specifically concerns the positivity of an “average entropy production”, $\langle \sigma \rangle$. Indeed, for the example parameters chosen in [1], this entropy production turns out to be positive at all times, cf. Fig 1. Consider, however, the following variation: Change all on-site potentials from $\omega = 1$ to $\omega = -50$. Since the model conserves particle numbers and the initial state has precisely five bosons, this only amounts to an energy shift of the full spectrum, i.e., adding original Hamiltonian. Hence,
The second claim addresses an integral fluctuation theorem which states \( \langle e^{-\sigma} \rangle = 1 \), where \( \sigma \) depends on the bath Hamiltonian and the full system state. Of course, at \( t = 0 \) the theorem holds by construction. In Fig. 2 we (re-)plot \( \langle e^{-\sigma} \rangle \) for the interaction strengths, \( \gamma' \), as addressed in [1] in the context of the integral fluctuation theorem, but add data also for the interaction strength \( \gamma' = 4 \), the latter is addressed in [1] only in the context of the afore mentioned entropy production. Again, we also plot the respective \( \langle n_0(t) \rangle \). Obviously, \( \langle e^{-\sigma} \rangle \approx 1 \) only holds to the extend to which the system remains in its initial state. Hence, the validity of the integral fluctuation theorem at short times is rather trivial. It breaks down as soon as the system “does something”, irrespec-

\[ \langle n_0(t) \rangle \]

\[ \langle e^{-\sigma} \rangle \]

\[ \gamma' \]

\[ \approx \]

\[ 1 \]

\[ t \]

\[ 2 \]

\[ 0001 010100 1000 \]

\[ 0.001 0.01 0.1 1 10 100 1000 \]

\[ 0 0.5 1 \]

\[ 0 0.5 1 \]

\[ -2 \]

\[ -2 \]

FIG. 1: (Color online) Time dependence of the (a) occupation probability \( \langle n_0 \rangle \) of the system site (any \( \omega \)), (b) average entropy production \( \langle \sigma \rangle \) for on-site potential \( \omega = 1 \) (original model), and (c) average entropy production \( \langle \sigma \rangle \) for on-site potential \( \omega = -50 \), at various interaction strengths \( \gamma' \).

FIG. 2: (Color online) Time dependence of the (a) occupation probability \( \langle n_0 \rangle \) of the system site (any \( \omega \)) and (b) “integral fluctuation quantity” \( \langle \exp(-\sigma) \rangle \) for on-site potential \( \omega = 1 \).

[1] E. Iyoda, K. Kaneko, and T. Sagawa, Phys. Rev. Lett. 119, 100601 (2017).

[2] S. Goldstein, J. L. Lebowitz, R. Tumulka, and N. Zanghi, Phys. Rev. Lett. 96, 050403 (2006).

[3] A. Riera, C. Gogolin, and J. Eisert, Phys. Rev. Lett. 108, 080402 (2012).

[4] J. Liphardt, S. Dumont, S. B. Smith, I. Tinoco Jr., and C. Bustamante, Science 296, 1832 (2002).

[5] C. B. Chiu, E. C. G. Sudarshan, and B. Misra Phys. Rev. D 16, 520 (1977).
Reply to arXiv:1712.05172

In the following we reply to the reply by E. Iyoda, K. Kaneko, and T. Sagawa (arXiv:1712.05172) to our previous comment on Phys. Rev. Lett. 119, 100601 (2017).

Iyoda et al. replied to a comment by Gemmer et al. on the arXiv. The paper at hand is our response to this reply. For completeness, we reprint below the text of in black lettering. We insert our responses to specific sections in green lettering. These responses conclude our discussion on the arXiv.

Gemmer et al. in their Comment make criticisms on our Letter, while they agree that our result is mathematically sound. Their arguments are summarized as (i) the Lieb-Robinson (LR) time \( \tau_{LR} \) is too short and “unphysical” for some examples, (ii) the average entropy production \( \langle \sigma \rangle \) becomes negative for some parameters, and (iii) in our numerical simulation, the integral fluctuation theorem (IFT) \( e^{-\gamma} = 1 \) holds only while the system remains in its initial state. Here we discuss that (i) and (ii) are not justified, but that (iii) is indeed a subtle point because of the large finite-size effect.

Comment to the previous section: The criticism in does not consist of three different points. It is essentially just one point, namely, that the range of the validity of the theorems in is physically extremely limited, rather than just not comprising “some examples”. This limitation, which arises from finite bath sizes, is neither discussed nor clearly stated in . Instead, a numerical example is presented to supposedly illustrate the validity of the theorems for relevant time scales. What is called points (ii) and (iii) above, are really only numerical observations, which elucidate that the theorems in are only trivially valid as long as the system does nothing.

Reply to (i). We agree that the LR times of their examples (proteins in water and coffee in air) are very short compared to their time scales (Brownian motion and daily life). However, these situations are clearly not relevant to our theory in , which is for isolated quantum systems where the bath is initially in a pure state (specifically an energy eigenstate). In fact, the setups discussed in are far from isolated and pure. In other words, in their setups the fluctuation theorem is not emergent from quantum mechanics, but is simply a consequence of the conventional scenario based on classical stochastic dynamics. Our result in implies that if air or water was initially in an energy eigenstate, then the IFT would hold only within such a very short time scale.

Intermediate comment: This is not correct: an IFT may still hold much longer due to alternative mechanisms, e.g., as suggested in .

We emphasize that our main focus is on ideally-isolated artificial quantum systems such as ultracold atoms, as explicitly stated in . In fact, the LR time is reasonably long for ultracold atoms, compared to the time scale of real experiments. For example, in a typical experiment , the experimental time scale is \( h/J \) and the LR time is \( \tau_{LR} \sim l^3/J \), where \( J \) is the tunneling amplitude and \( l \) is the side length of \( B_1 \) in .

Comment to the previous section: The conceptual framework of the paper is that of quantum typicality, the eigenstate thermalization hypothesis, and Lieb-Robinson bounds. The first two concepts are notable and relevant precisely because they potentially explain fundamental features of thermodynamical behavior (like equilibration and thermalization) for the full range of systems, i.e., from microscopic ultracold atom experiments all the way to macroscopic daily life physics such as cups of coffee. As cited in , a number of statements in imply the same validity range and impact for the findings in . Here we quote yet another on. In the introduction of it reads: “In this sense, a fundamental gap between the microscopic and the macroscopic worlds has not yet been bridged: How does the second law emerge from pure quantum states?” We leave it to the reader to decide whether the fact that the results of are truly conceptually limited to specific possible future ultracold atom experiments is made sufficiently transparent in .

Reply to (ii). The reason why the authors of observed the negative entropy production for some parameters is that their choice of the initial eigenstate is not thermal for such cases, as detailed below. We note that our theory states that the second law and the IFT hold if the initial eigenstate is thermal.

In the hard-core boson model in , the total Hilbert space of bath \( B \) is divided into particle-number sectors, labeled by \( N \). An energy eigenstate is thermal only if it is in a sector whose \( N \) is close to the average particle number \( N^* \) in the canonical ensemble, because the strong eigenstate thermalization hypothesis (ETH) is valid only within each particle number sector . We note that the weak ETH is true without dividing the energy shell to particle-number sectors. Because \( N^* \simeq 15.9 \) with \( \omega = -50 \) and \( \beta = 0.1 \), the choice of \( N = 4 \) in is far from \( N^* \), which makes the initial eigenstate athermal.

To directly show this, we calculated the trace norm between the reduced density operators of an energy eigenstate \( |E_i \rangle \) and the corresponding canonical ensemble: \( \delta_{tr} := ||\text{tr}_{B_2}(|E_i \rangle \langle E_i |)| - \text{tr}_{B_2}[\rho_{B_2,\text{can}}]||_1 \). Figure 1 shows the \( N \)-dependence of \( \delta_{tr} \), where we take \( B_2 \) as the \( 2 \times 2 \) lower-left sites of bath \( B \). As shown in Fig. 1, \( \delta_{tr} \) takes a smaller value when \( N \) is closer to \( N^* \). For \( \omega = -50 \) and \( N = 4 \) (red circle), \( \delta_{tr} \) is large and \( \langle |E_i \rangle \rangle \) is not at all thermal.

We have also confirmed that the entropy production is positive for a broad range of parameters, as long as the initial eigenstate is thermal. We calculated \( \langle \sigma \rangle \) at \( t = \tau_{LR} \) for \( \omega = \pm 1, \pm 2, \pm 4, \pm 5, \pm 16, \pm 32, -50 \), \( \beta = 0.1, 0.3 \), \( \gamma = 0.05, 0.1, 0.4, 1.0, 4.0, g = 0.1, 0.4 \), and \( N = 4 \). We found that \( 0.0076 \leq \langle \sigma \rangle \leq 1.84 \) if \( \delta_{tr} < 0.3 \) (thermal), while \( -8.86 \leq \langle \sigma \rangle \leq 0.095 \) if \( \delta_{tr} > 1.7 \) (athermal).
In [3], we concluded that the IFT non-trivially holds in short time regimes. The reply at hand by Iyoda et al. surprisingly argues based on the fact that the quantitative error evaluation, scaling of $\propto t^2$, is consistent with the prediction by the LR argument (the inset of Fig. 3 in [3]). On the other hand, the authors of [3] argued that this scaling is just a general property of quantum systems.

FIG. 3: The $N$-dependence of $\delta_{tr}$. The Hamiltonian and the lattice are the same as in [2]. The parameters are given by $\omega = 1, 8, -50$, $g = 0.1$, and $\beta = 0.1$. $N^{\omega=1}_c$ and $N^{\omega=-8}_c$ are the average particle numbers in the canonical ensemble for $\omega = 1, 8$, respectively. For each data point, 10 energy eigenstates are sampled, and the error bar represents their standard deviation. The red circle indicates the parameters used in [2] ($\omega = -50$ and $N = 4$). The blue circle indicates the parameters used in [2] ($\omega = 1$ and $N = 4$).

Comment to the previous section: While a numerical agreement with the IFT would be remarkable because it is requires $\langle \exp(-\sigma) \rangle$ to equal precisely unity, an agreement with the “entropy production theorem” is much less remarkable, even for a “broad range of parameters”, since it only requires $\langle \sigma \rangle$ to be non-negative. The latter may simply occur by chance, cf. below. Furthermore, as the title indicates, [3] is primarily about the fluctuation theorem, rather than about the much weaker positivity of entropy production.

First of all, the reply at hand by Iyoda et al. indicates that “thermality” of the initial state acutely requires an involved fine tuning of model parameters that may possibly work out at some specific instance. This appears to be true even in the limit of infinitely large baths. Again, we leave it to the reader to decide whether this fact is clearly communicated in [3].

Moreover, in the original paper [3] the error bound for the entropy production theorem is given by $\epsilon_{2nd}$ [Eq.(3)]. In the reply at hand Iyoda et al. surprisingly argue based on the smallness of a parameter $\delta_{tr}$ which does not even appear in the original paper. Apparently, $\delta_{tr}$ has to be small to guarantee “thermality” of the initial state. It is, however, entirely unclear how small $\delta_{tr}$ has to be to indicate sufficient thermality. In the reply at hand Iyoda et al. classify (without further justification) $\delta_{tr} < 0.3$ (thermal) and $\delta_{tr} > 1.7$ (athermal). While the example in [2] ($\omega = -50, N = 4$) yields $\delta_{tr} \approx 2$ and thus barely results as “athermal”, the original example in [3] ($\omega = 1, N = 4$) yields $\delta_{tr} \approx 0.7$ (blue circle in Fig. 1), i.e., does not qualify as “thermal” either, according to the above ad hoc classification. Given that $\delta_{tr}$ is meant to quantify the distance of the local initial bath state from a true thermal state, it should, to be a bit more quantitative, at least be compared to the corresponding norm of the thermal state itself. The latter equals unity (i.e., the 1-Schatten-norm of a density matrix). So for “closeness” to the thermal state one should require $\delta_{tr} \ll 1$. This, however, is hardly reached anywhere in all the many parameter combinations displayed in Fig. 1, and surely not for the original example (blue circle). This suggests that, due to the bath being far too small, the presented model is for no parameter setting really within the regime of validity of the proclaimed theorem and the positivity of the entropy production is a coincidence which is not truly enforced by the validity of the theorem.

Reply to (iii). In [3], we concluded that the IFT non-trivially holds in the short time regime based on the fact that the quantitative error evaluation, scaling of $\propto t^2$, is consistent with the prediction by the LR argument (the inset of Fig. 3 in [3]). On the other hand, the authors of [3] argued that this scaling is just a general property of quantum systems.

After careful consideration with some additional numerical simulation, we have to admit that it is hard to conclude whether the $t^2$-scaling comes from the LR argument or not based on our numerical data, because the finite-size effect is very large within the numerically-accessible system size. We expect, however, that the IFT can be verified more clearly by using ultracold atoms, with which the system size can be much bigger than numerics. We note that the time range where the IFT holds will linearly increase with $l$. If one can take $l \sim 10^2$, the LR time becomes a hundred times of the experimental time scale, which can be realized with the current or the near-future technologies.

In addition, we remark that $|\gamma'|$ should not be taken too large to verify the IFT, because the larger $|\gamma'|$ is, the more the condition (8) in [3] is violated. In this respect, the emphasis in [3] on the failure of the IFT for $\gamma' = 4$ is misleading.

Comment to the previous section: The justification of the fluctuation theorem is the major content of [3] as already the title indicates. Iyoda et al. present a numerical example (instead of a discussion of actual finite bath sizes) to support the applicability of the theorem. In [2], we demonstrated that the theorem only holds if the system does nothing. We further argued that a quadratic time dependence of $\langle \exp(-\sigma) \rangle$ does not indicate the validity of the theorem. In the reply at hand Iyoda et al. admit that a quadratic time dependence of $\langle \exp(-\sigma) \rangle$ does not indicate the validity of the theorem. However, they do not comment at all on the fact that the theorem only holds as long as the system does nothing. But this is the most important point. As long as this point stands, the numerical example does not support...
the applicability and relevance of the theorem in any way. (As opposed to the statement in the abstract of \cite{3} (literal quotation): “We confirmed our theory by numerical simulation of hard-core bosons, and observed dynamical crossover from thermal fluctuations to bare quantum fluctuations”). Since, to repeat, the regime of applicability of the theorem is extremely narrow, this finding is hardly surprising. It only concretely reflects the general fact that the range of validity of the proclaimed theorem is very small compared to the factually immensely large applicability of the second law or fluctuation theorems. This is true irrespective of any hypothetical models or possible future experiments on cold atoms.

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[7] The blue circle has been added to Fig. 1 by J. Gemmer, L. Knipschild, and R. Steinigeweg, for better visibility.