Enhancing violations of Leggett-Garg inequalities in nonequilibrium correlated many-body systems by interactions and decoherence

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We identify different schemes to enhance the violation of Leggett-Garg inequalities in open many-body systems. Considering a nonequilibrium archetypical setup of quantum transport, we show that particle interactions control the direction and amplitude of maximal violation, and that in the strongly-interacting and strongly-driven regime bulk dephasing enhances the violation. Through an analytical study of a minimal model we unravel the basic ingredients to explain this decoherence-enhanced quantumness, illustrating that such an effect emerges in a wide variety of systems.

For several decades, assessing the existence of genuine quantum behavior and quantifying coherence in quantum systems have remained as fundamental open problems, critical to applications in computation and information processing. A seminal breakthrough in this direction was made by Leggett and Garg, who considered the conditions that a macroscopic system entirely described by classical physics should satisfy. These are macroscopic realism (a system's property is well defined at every time regardless of whether it is observed or not) and noninvasive measurability (the system is unaffected by measurements on it). When these conditions are met, the system satisfies the so-called Leggett-Garg inequalities (LGIs). The experimental observation of their violation, which serves as witness of quantum coherence, has been sought intensively and reported in various platforms.

In order to establish realistic conditions where LGIs are maximally violated, providing optimal settings for quantum protocols performed in a particular system, its unavoidable coupling to the environment has to be considered. Recent theoretical research on few-qubit systems has determined that Markovian noise degrades quantumness, while non-Markovianity helps restore it. However, many-body interacting systems, where spectacular effects resulting from quantum coherence emerge, remain unexplored within this effort. The non-trivial impact of dissipation in multilevel systems is known to induce unexpected beneficial effects, as entanglement generation and quantum state engineering, restoration of hidden quantum phase transitions and environment-assisted transport, recently observed in several quantum simulators. Thus such systems constitute attractive candidates for uncovering novel mechanisms of LGI violation enhancement.

In the present work we establish such mechanisms in testbed open many-body systems. We show that not only particle interactions, but also bulk dephasing, can increase the violation of LGIs in Markovian systems. For this we assess the quantumness of the transport supported by interacting spin chains when driven out of equilibrium by unequal boundary reservoirs, a configuration considered so far for LGIs on single-particle systems only.

Using a minimal model to illustrate the basic ingredients responsible for this phenomenon, we argue that it can emerge under a wide range of conditions.

Methods

Nonequilibrium setup. We consider a spin-1/2 chain coupled to two reservoirs of unequal magnetization at its boundaries, as depicted in Fig. 1. These induce a net homogeneous spin current in its nonequilibrium steady state (NESS). The chain is characterized by the one-dimensional XXZ Hamiltonian

\[ \hat{H} = \tau \sum_{n=1}^{L-1} \left[ \hat{\sigma}_n^x \hat{\sigma}_{n+1}^x + \hat{\sigma}_n^y \hat{\sigma}_{n+1}^y + \Delta \hat{\sigma}_n^z \hat{\sigma}_{n+1}^z \right], \]
where $\hat{\sigma}_\alpha$ are the Pauli matrices ($\alpha = x, y, z$), $L$ is the number of sites, $\tau$ is the exchange interaction (we set the energy scale by taking $\tau = 1$), and $\Delta$ is the anisotropy along $z$ direction; we take $\Delta \geq 0$ without loss of generality. When mapping the model to a spinless-fermion description, $\tau$ corresponds to the hopping and $\Delta \tau$ to a density-density interaction; thus $\Delta > 1$ is referred to as the strongly-interacting regime.

The boundary reservoirs are modeled as noninteracting spin chains with different average magnetizations. In addition, both are weakly coupled to the XXZ chain, and their time correlations decay very rapidly, so their memory effects can be neglected (Markov approximation). Furthermore, the so-called wide-band limit is considered, where the bandwidths of the reservoirs, proportional to their hopping rates, are much larger than the bandwidth of the XXZ chain. Invoking these assumptions and following standard microscopic derivations where the degrees of freedom of the reservoirs are traced out, it is shown that the dynamics of the chain under the influence of the environment is governed by a Lindblad master equation,

$$\dot{\rho} = \hat{L}(\rho) = -i[H, \rho] + \sum_{k} \hat{V}_k \rho \hat{V}_k^\dagger - \frac{1}{2} \{\hat{V}_k, \hat{V}_k^\dagger\}.$$  \hspace{1cm} (2)

Here $\rho$ is the density matrix of the chain, $\hat{L}$ is the Lindblad superoperator, $\{.,.\}$ is the anticommutator of two operators, and $\hat{V}_k$ correspond to the jump operators establishing the coupling of the chain to the environment. For the boundary driving we consider operators that annihilate (creates) spin excitations at both the left ($l$) and right ($r$) edges of the chain, given by $\hat{V}_{l,r} = \sqrt{\Gamma(1 \mp f)} \hat{\sigma}_{l,r}^z$ and $\hat{V}_{l,r}^\dagger = \sqrt{\Gamma(1 \pm f)} \hat{\sigma}_{l,r}^x$. Here $\Gamma$ is the coupling strength (we take $\Gamma = 1$), and $\pm f$ are the average magnetizations per spin in dimensionless units of the left/right reservoirs. Thus the parameter $f$ ($0 \leq f \leq 1$) is the driving, as it establishes the magnetization imbalance between the boundaries. If $f = 0$, spin excitations are created and annihilated at the same rate on both boundaries, so there is no net magnetization imbalance and thus no spin transport. If $f > 0$, more excitations are created (annihilated) on the left-most (right-most) site of the lattice, inducing a net current resulting from a left-to-right flow and its weaker backflow. We also consider bulk dephasing processes, arising from the coupling of every site of the XXZ chain to local harmonic vibrational degrees of freedom corresponding to the oscillation of the lattice, and quantized in terms of linear phonons. Tracing out these degrees of freedom, and considering the wide-band limit, the resulting jump operators are $\hat{V}_{l,r} = \gamma \tau \hat{\sigma}_n^z$ ($n = 1, \ldots, L$), where $\gamma$ is the homogeneous dephasing rate.

When the spin chain evolves in time as dictated by Eq. (2), it eventually reaches its unique NESS, given by $\hat{\rho}_{\text{NESS}} = \lim_{t \to \infty} \hat{\rho}(t) = \lim_{t \to \infty} \exp[\hat{L}(t)]\hat{\rho}(0)$, with $\hat{\rho}(0)$ an initial state. Its transport properties are characterized by its magnetization profile $\langle \hat{\sigma}_z \rangle$ and the homogeneous spin current $J = \langle \hat{J} \rangle$, with $\hat{J}_n = 2(\hat{\sigma}_n^x \hat{\sigma}_{n+1}^x - \hat{\sigma}_n^y \hat{\sigma}_{n+1}^y)$. The phase diagram of the dephasing-free model, obtained from the behavior of both quantities, is depicted in Fig. 1. For weak driving $f$ (linear response), $\Delta < 1$ shows ballistic conduction while for $\Delta > 1$ the system satisfies a normal diffusion equation. This indicates a nonequilibrium quantum phase transition at the isotropic point $\Delta = 1$, which is super-diffusive. For large driving $f$ and $\Delta > 1$, negative differential conductivity (NDC) emerges, leading to an insulating state at maximal driving $f = 1$ in which opposite-polarized ferromagnetic domains suppress transport. In the presence of dephasing, spin transport is monotonically degraded with $\gamma$ and becomes diffusive for $\Delta < 1$, while it is largely enhanced with $\gamma$ for $\Delta > 1$, a manifestation of strong correlations. The enhancement vastly increases with driving, as dephasing washes out the NDC and induces an insulator-conducting transition at $f = 1$.

**Results**

**Leggett-garg inequalities calculation.** As shown by Leggett and Garg, macroscopic classical systems satisfy the inequality $\mathcal{C}(t_1, t_2) + \mathcal{C}(t_2, t_3) - \mathcal{C}(t_1, t_3) \leq 1$ ($t_1 < t_2 < t_3$). Here $\mathcal{C}(t_1, t_2)$ denotes the two-time correlations of a dichotomic operator $\hat{Q}$ (with eigenvalues $\pm 1$) between times $t_1$ and $t_2$, and is given by $\mathcal{C}(t_1, t_2) = \frac{1}{4} \langle \{\hat{Q}(t_1), \hat{Q}(t_2)\} \rangle$. For the NESS $\hat{\rho}_{\text{NESS}}$, which is unaffected by an evolution under $\hat{L}$, this correlation with $t_1 < t_2$ is given by...
Figure 2. Time correlations \( C_\alpha(t) \) (a,b) and Leggett-Garg functions \( \mathcal{K}_\alpha(t) \) (c,d) as a function of time and anisotropy \( \Delta \) for weak driving \( f = 0.1 \) and system size \( L = 60 \). (a,c) \( \alpha = x \), (b,d) \( \alpha = z \). The qualitative behavior for \( \Delta = 0 \) is very close to an identity (with terms of higher-order corrections for correlations), the results are very well approximated by known analytical results for an infinite-temperature state. These correspond to an exponential decay for \( \Delta < 1 \) to diffusive \((\Delta > 1) \) spin transport. First, since for \( \Delta = 0 \) and weak driving the NESS is very close to an identity \((-\Delta \leq 1) \), the LGI reduces to \( \mathcal{K}(t) \equiv 2(C(t) - C(2t)) \leq 1 \), where we define the Leggett-Garg function \( \mathcal{K}(t) \), and \( \mathcal{C}(t) \equiv C(0,t) \). Note that we cannot regard the nature of transport as classical from observing that the LGI for some \( Q \) is satisfied, as it might not capture the quantum correlations that inequalities for other measurements might. However, we do assess genuine quantum behavior when one LGI is violated.

We focus on LGIs when performing measurements of local observables \( \hat{Q} = \hat{\rho}_l^\alpha (\alpha = x,z) \) for site \( l = L/2 \) on the NESS \( \hat{\rho}_\infty \). In this form we reduce edge effects as much as possible; however we have verified that the results are qualitatively the same when performing the measurements on different sites (see Fig. S2 of the Supplementary Information). To evaluate the LGIs violation in the boundary-driven setup for large systems, we obtain their NESS applying the time-dependent density matrix renormalization group \(^{43,44}\) (See Supplementary Information). To calculate the LGIs, we define the Leggett-Garg function \( \mathcal{K}(t) \) follows immediately. Our simulations are based on the open-source Tensor Network Theory (TNT) library \(^{46,47}\). This constitutes a novel and topical application of matrix product states, fueled by the growing interest in evaluating two-time correlations in dissipative many-body systems \(^{48-52}\).

Controlling LGI violations with interactions: dephasing free case. We now show that violations of LGIs can be tuned by interactions, and can indicate nonequilibrium quantum phase transitions. For this we consider the linear-response regime, where the system presents a transition from ballistic \((\Delta < 1) \) to diffusive \((\Delta > 1) \) spin transport. In Fig. 2(a,b) we show \( C_\alpha(t) \) for \( \alpha = x,z \), which measure the response of the system when adding or removing a spin excitation for \( \alpha = x \), or measuring the local magnetization for \( \alpha = z \). These correlations already show a qualitative difference, most notable for early times, between the two transport regimes. First, since for \( \Delta = 0 \) and weak driving the NESS is very close to an identity \((-\Delta \leq 1) \), the LGI reduces to \( \mathcal{K}(t) \equiv 2(C(t) - C(2t)) \leq 1 \), where we define the Leggett-Garg function \( \mathcal{K}(t) \), and \( \mathcal{C}(t) \equiv C(0,t) \). Note that we cannot regard the nature of transport as classical from observing that the LGI for some \( Q \) is satisfied, as it might not capture the quantum correlations that inequalities for other measurements might. However, we do assess genuine quantum behavior when one LGI is violated.

Thus, \( \mathcal{C}(t_1, t_2) = \text{Re}(\text{Tr}[\hat{Q} \exp(\hat{L}(t_1 - t_2)\hat{\rho}_\infty)]) \). (3)

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\( ^a \)We do not consider longer times, where revivals of the LGI violations occur, as we are mostly interested in the maximal violations \( \mathcal{K}_{\text{Max}} \) which take place at an early time.
This also shows that the LGI violation indicates the nonequilibrium critical point, a property that it also features in equilibrium. 

**Dephasing-enhanced LGI violations.** Now we discuss LGIs of the driven system in the presence of bulk dephasing. As previously mentioned, for strong interactions $\Delta > 1$ and large driving $f = 1$ dephasing melts the ferromagnetic domains that suppress transport, inducing a transition to a conducting state. Thus the spin current is enhanced with $\gamma$ by several orders of magnitude, as shown in Fig. 4(a). This constitutes a many-body scheme of environment-assisted transport. Here we calculate the maximum violation of the LGI for $\alpha = z$ as a function of $\gamma$, also shown in Fig. 4(a). Small systems are considered to be able to calculate the NESS in the absence of (or for very weak) dephasing, which takes an exponentially-long time due to the presence of the ferromagnetic domains.

For $\gamma = 0$ LGIs are markedly violated, since operator $\hat{Q}$ is applied between the ferromagnetic domains and induces appreciable dynamics. But remarkably, as the system becomes conducting due to weak dephasing, it also presents enhanced quantumness measure manifested in the increase of the violations. Even for stronger dephasing $\gamma \approx 1$, where $K_{\text{Max}}$ decreases with $\gamma$, the violation is still larger than that of $\gamma = 0$. Thus there is a wide range of environmental couplings where in addition to a large transport enhancement, quantum features are strengthened. This is in stark contrast to the weakly-interacting case, depicted in Fig. S1 of the SI (See Supplementary Information), where both the spin transport and the violation of LGIs are monotonically degraded with dephasing. This indicates that the origin of the observed effect is truly a consequence of strong interactions between particles, a scenario where LGIs remain largely unexplored.

We also observe enhanced violation of LGIs with dephasing even for much weaker driving $f$, where for $\gamma = 0$ the system is conducting and the differential conductivity is positive (as NDC emerges at larger driving). In Fig. 4(b) we present the maximal violation as a function of $\gamma$ for $\Delta = 2$ and an intermediate driving $f = 0.5$, in which the system is conducting and far away from the insulating limit. We first note that in the absence of dephasing, the violation for $f = 0.5$ is larger than that at $f = 1$ (see Fig. 4(a)), which shows that just making the system conducting by inducing a magnetization backflow increases the quantumness measure in the lattice. Furthermore,
when dephasing is included, it increases the violation compared to the $\gamma = 0$ case; this indicates that the effect is not just a peculiarity of the maximally-driven limit, but emerges in a broader transport regime. The key ingredient is again the existence of strong interactions $\Delta$. This strongly contrasts with the natural expectation that in conducting regimes, environmental coupling degrades LGI violations.

It is important to stress two additional properties evidenced in Fig. 4(b). First, the maximal violation barely changes with the system size, indicating that this is not a small-lattice effect. We have performed simulations around the optimal dephasing rate for systems of up to $L = 150$, and observed that $\mathcal{K}_{\text{Max}}$ slightly increases with $L$, from $\mathcal{K}_{\text{Max}} = 1.116$ for $L = 30$ to $\mathcal{K}_{\text{Max}} = 1.120$ (not shown). Thus for large systems the positive impact of dephasing is still present and of almost the same amplitude of that at much smaller lattices. Second, the optimal dephasing slightly shifts to higher values with $L$, but for the largest chains considered, it remains $\approx 0.10$. This leads to a wide range of dephasing rates for which the LGI violation is larger than that of the $\gamma = 0$ limit.

Finally, we note that the LGI violation enhancement by dephasing is also observed when non-local observables $\hat{Q}$ are considered. In particular, we calculated the two-time correlations for strings of operators $\hat{Q} = \hat{\sigma}_x^{(1)} \hat{\sigma}_x^{(2)} \cdots \hat{\sigma}_x^{(L)}$ of different length, located around the center of the XXZ lattice. The results, shown of Fig. S3 of the SI (See Supplementary Information), are very similar to those of Fig. 4, both at and away from strong driving, where the maximal LGI violation takes place at a finite dephasing rate. This makes our conclusions more robust, and suggests that this phenomenon could be observed in experiments where measurements are performed on a non-local basis.

Minimal model. To obtain more insight into the incoherent enhancement of LGI violations, we analyze a simple model which incorporates the essential ingredients of the strongly-interacting lattice. This model, depicted in Fig. 5, mimics its gapped eigenstructure, consisting of flat (insulating) and wide (conducting) bands, and the population transfer between them due to coherent processes, incoherent driving and dephasing. It consists of $K$ levels $|1\rangle, \ldots, |K\rangle$, with Hamiltonian

$$\hat{H}_{\text{Min}} = \frac{1}{2} \sum_{k=1}^{K-1} (|k\rangle \langle k+1| + \text{H.c.}) + \delta |K\rangle \langle K|,$$

where state $|K\rangle$ is elevated in energy with respect to the others by an amount $\delta > 0$; thus the bands are separated by a gap of $O(\delta)$, similarly to the strongly-interacting XXZ model (gaps of $O(\Delta)$). The driving is modeled by the incoherent coupling of states $|1\rangle$ and $|K\rangle$ to an auxiliary site $|s\rangle$, with jump operators $\hat{V}_{k,s} = \sqrt{1 + f} \hat{\Lambda}_{k,s}$ and $\hat{V}_{s,k} = \sqrt{1 + f} \hat{\Lambda}_{s,k}$, where $\hat{\Lambda}_{k,s} = |s\rangle \langle k+1|$. In addition, the dephasing at rate $\gamma$ corresponds to the jump operator $\hat{\Lambda}_z = \sqrt{2} (\hat{I} - 2 |K\rangle \langle K|)$, with identity $\hat{I}$, which is equivalent to $\hat{\delta}^2$ in the XXZ model and acts only on the state of highest energy. This is similar to the effect of dephasing on the original many-body system, which induces transitions from high-energy flat bands of the eigenstructure to low-energy wide bands of higher conduction. Finally, the associated local current operator is $\hat{I}_{\text{Min},k} = -i(|k\rangle \langle k+1| - \text{H.c.})$.

This model leads to the emergence of NCD, an insulating state at $f = 1$ and dephasing-enhanced transport. These effects are shown in Fig. 6(a) for $K = 10$, $\Gamma = 1$ and $\delta = 1$. Note that $\delta = 1$ does not correspond to the isotropic point of the XXZ model. The model does not capture the transport phase transition, as it is defined to mimic the strongly-interacting regime of the spin chain. Here $\delta$ sets the size of the gap between bands. We clearly see that when $\gamma = 0$ the system is insulating at maximal driving $f = 1$, where the equivalent of the ferromagnetic domains is a preferred population of state $|K\rangle$ (see Eq. (S1) of the SI). The NDC is washed out by dephasing, which results in a large transport enhancement with $\gamma$. For large dephasing the transport is degraded, as a result of the Zeno effect which tends to freeze the dynamics. Thus the main transport properties of the strongly-interacting XXZ system are captured by the minimal model.
To study LGIs, we calculate the time correlations for the operator $\hat{Q} = 2|P\rangle\langle P|$ where site $P$ is taken on the central site of the system. Exact numerical results of the Leggett-Garg function $k(t)$ are depicted in Fig. 6(b), showing that, similarly to the original model, two mechanisms enhance the violations of LGIs with respect to the dephasing-free $f = 1$ limit (where there is no visible violation), namely introducing a backflow ($f < 1$) or dephasing ($\gamma > 0$). Very large dephasing degrades this scenario, as expected. Thus in spite of its simplicity, the model features the essential ingredients underlying such phenomena.

Analytical results up to $O(\delta^2)$ for the strongly-driven limit, where the effects of decoherence are the largest, help determine how LGI violations are increased; see details in the SI (See Supplementary Information). For the dephasing-free system with $f = 1$, $C^{(0)}(t) \approx K^{(0)}(t) \approx 1$, so the LGI is not significantly violated, as expected. Defining $\beta = 2(1 - f)(1 + \Gamma^2)$ when slightly moving from maximal driving with $\gamma = 0$, or $\beta = 16\gamma(1 + \Gamma^2)/\Gamma$ when introducing weak dephasing at $f = 1$, or their sum if both are present, we get the general behavior

$$k(t) = 1 + \frac{\beta}{\Gamma} \left( 1 - e^{-\gamma t} \right)^2.$$  

This shows that both mechanisms induce an appreciable violation of the LGI which grows quadratically at early times, and which increases linearly as $(1 - f)$ and/or $\gamma$. It also manifests that the source of these results, also present in the strongly-interacting XXZ model, is the gapped eigenstructure of the model.

### Discussion

We have discussed schemes for increasing violations of Leggett-Garg inequalities in open many-body systems, illustrated in archetypical nonequilibrium boundary-driven configurations. Using matrix product state simulations, we have determined that in the strongly-interacting regime, interactions and (unexpectedly) bulk dephasing can enhance the violations. The main mechanism behind the latter effect is illustrated by the same observation introduced37,38) current-carrying systems. We have discussed schemes for increasing violations of Leggett-Garg inequalities in open many-body systems, illustrated in archetypical nonequilibrium boundary-driven configurations. Using matrix product state simulations, we have determined that in the strongly-interacting regime, interactions and (unexpectedly) bulk dephasing can enhance the violations. The main mechanism behind the latter effect is illustrated by the same observation.

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Author contributions

J.J. Mendoza-Arenas developed the theoretical framework and implemented the time evolution codes. F.J. Gómez-Ruiz developed numerical simulations and prepared the figures. All authors contributed to the analysis of the results and the writing of the manuscript. L. Quiroga and F.J. Rodriguez supervised the project.

Competing interests

The authors declare no competing interests.

Additional information

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