

Mixed state entanglement via the Cauchy-Schwarz inequality

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(Received 3 August 2025; revised 9 May 2026; accepted 6 July 2026; published 23 July 2026)

The entanglement properties of mixed states are of great importance in the study of open quantum systems and quantum information science, but common entanglement criteria such as the Peres-Horodecki condition can be difficult to relate to physical properties of the system. We introduce the Cauchy-Schwarz violation (CSV) condition for entanglement, which has a simple dependence on the populations and coherences of the density operator. A sufficient condition for entanglement, it provides a direct connection to the physical characteristics of the system such as its symmetries, yielding intuition that can be used to understand and engineer highly entangled states. We illustrate the often surprising insights gained from the CSV condition by applying it to the Jaynes-Cummings model, the quantum Rabi model, and an open-system quantum Rabi model.

DOI: 10.1103/3s44-6j39

Since its introduction nearly a century ago [1], quantum entanglement has attracted great interest for its importance in quantum computing and information science [2,3], its significance as a fundamental difference between quantum and classical mechanics [4–6], and its possible influence on chemical processes [7–10]. Several approaches have emerged to characterize the entanglement of mixed states [11,12], including the Peres-Horodecki criterion [13,14], which states that a density operator ρ is entangled if its partial transpose ρ^{PT} is not positive semidefinite. Though widely used [15–17], this condition can be challenging to interpret physically due to the generally complex relationship between eigenvalues and physical features like populations, coherences, and symmetries. Developing such physical insight is crucial for applications such as engineering Hamiltonians and system-environment interactions that produce highly entangled steady states robust against dissipation.

In this Letter, we introduce a characterization of entanglement directly dependent on populations and coherences, establishing immediate connections between entanglement and physical structure. We apply this approach to the Jaynes-Cummings model (JCM) and quantum Rabi model (QRM), demonstrating its simplicity as well as the connections it establishes between symmetry and entanglement. These principles generalize to larger systems, suggesting that this approach provides a useful perspective on entanglement complementary to that provided by standard entanglement monotones.

The CSV condition. To develop an alternative to the Peres-Horodecki criterion, we seek a simple way to test whether an operator is positive semidefinite. By Sylvester’s criterion, an $n \times n$ Hermitian matrix A is positive semidefinite if and only if all principal minors are non-negative [18]. In the context of the density operator ρ , each minor serves as a “source” of nonpositive semidefiniteness (hence entanglement), with the minors of larger submatrices representing more delocalized entanglement involving many populations and coherences. As a tractable estimate, we focus on the localized sources of entanglement, arising from the principal minors associated with the smallest submatrices. 1×1 submatrices of ρ^{PT} automatically give non-negative principal minors, so the first possibility of entanglement comes from the 2×2 submatrices. The minor involving rows i and j is non-negative if $\rho_{ii}^{\text{PT}} \rho_{jj}^{\text{PT}} \geq |\rho_{ij}^{\text{PT}}|^2$, so a system must be entangled if it violates this inequality for some i and j . Because this condition equivalently follows from the Cauchy-Schwarz inequality [19–21], we refer to this test of entanglement as the Cauchy-Schwarz violation (CSV) condition. This condition is a sufficient, but not necessary, condition for both ρ^{PT} to not be positive semidefinite and the system to be entangled.

Although we have written the CSV criterion in terms of ρ^{PT} , it is ultimately a comparison of the populations and coherences of the original physical density operator ρ . This transparent connection to populations and coherences makes the CSV condition amenable to simple qualitative analysis. This will be illustrated in the next section where the condition will be used to connect symmetry and entanglement without needing explicit numerical computations, something that is difficult to achieve with a less physically intuitive condition like Peres-Horodecki or entanglement witnesses [22,23]. By not requiring numerics, the CSV approach allows for a physical, rather than solely computational, understanding of entanglement.

To quantify the degree to which the Cauchy-Schwarz inequality is violated, we introduce the quantity $S(\rho) = \sum_{i>j} \max\{|\rho_{ij}^{\text{PT}}|^2 - \rho_{ii}^{\text{PT}} \rho_{jj}^{\text{PT}}, 0\}$, analogous to the negativity

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$\mathcal{N}(\rho) = \sum_{\lambda_k \in \text{spec}(\rho^{\text{PT}}), \lambda_k < 0} |\lambda_k|$, which is a quantification of the Peres-Horodecki condition [24]. In what follows, $\mathcal{S}$ will serve as a simple way to visualize our physical arguments about coherences and their effect on the Cauchy-Schwarz violation. The precise numerical value of $\mathcal{S}$ is less important: Indeed, $\mathcal{S}$ can be zero in one product basis but nonzero in another (and hence it is not an entanglement monotone). Nonetheless, this does not limit the insights gained from the CSV condition: Once one chooses a fixed, physically relevant basis, where the behavior of coherences can be intuitively understood, the CSV condition translates that intuition into information about entanglement.

The Sylvester criterion shows rigorously that $\mathcal{S}(\rho) > 0$ implies $\mathcal{N}(\rho) > 0$; however, one intuitively also expects that a larger value of $\mathcal{S}$ (in a fixed basis) corresponds to a larger value of $\mathcal{N}$. At present, we do not make this correspondence mathematically precise, but we will show that it holds for several examples below. This will suggest that the CSV condition is a useful tool not only for physically understanding whether or not a system is entangled, but also for quantifying how much entanglement is present.

Application: low-temperature Jaynes-Cummings and quantum Rabi models. To illustrate the general principles of the CSV approach, we compare the entanglement of the JCM and QRM, two models of a two-level system (TLS) interacting with a bosonic mode [25–36]. This will demonstrate both the correlation between the magnitudes of $\mathcal{S}$ and $\mathcal{N}$ and the connection between symmetry and entanglement provided by the CSV condition. The QRM is given by the Hamiltonian $H_{\text{QRM}} = \frac{\Delta}{2}\sigma_z + a^\dagger a + \lambda\sigma_x(a + a^\dagger)$, with σ_z, σ_x Pauli matrices and $a^\dagger$ (a) the creation (annihilation) operator for a bosonic mode. The JCM is obtained from the QRM by discarding counterrotating interaction terms to yield $H_{\text{JCM}} = \frac{\Delta}{2}\sigma_z + a^\dagger a + \lambda(\sigma^- a^\dagger + \sigma^+ a)$, with $\sigma^\pm$ the TLS raising/lowering operators. The JCM conserves the excitation number $N = (\sigma_z + 1)/2 + a^\dagger a$, while the QRM only has a $\mathbb{Z}_2$ symmetry, conserving the parity $P^{\mathbb{Z}_2} = -\sigma_z(-1)^{a^\dagger a}$ of the total excitation count.

Consider first the low-temperature thermal states of the JCM, which can be solved exactly (see Sec. 1 of the Supplemental Material [37]), providing an opportunity to analytically validate the CSV approach. One finds an infinite sequence of coupling values $\lambda_0 < \lambda_1 < \lambda_2 < \dots$, such that when $|\lambda| \in (\lambda_{n-1}, \lambda_n)$, there is a unique ground state $|G(\lambda)\rangle$ with n excitations, while for $|\lambda| = \lambda_n$, the ground state is twofold degenerate, with one state $|G_1(\lambda)\rangle$ having n excitations and the other $|G_2(\lambda)\rangle$ having $n+1$. Consequently, in the zero-temperature limit, the thermal state $\rho_{\text{Th}} = e^{-\beta H}/Z$ is of the form $\rho_{\text{Th}} = |G(\lambda)\rangle\langle G(\lambda)|$ when $|\lambda| \in (\lambda_{n-1}, \lambda_n)$, and $\rho_{\text{Th}} = \frac{1}{2}(|G_1(\lambda)\rangle\langle G_1(\lambda)| + |G_2(\lambda)\rangle\langle G_2(\lambda)|)$ otherwise.

From this structure of the thermal state, dictated by excitation number symmetry, one can qualitatively understand thermal entanglement through the CSV condition. When $|\lambda| \in (\lambda_{n-1}, \lambda_n)$ for some n , ρ_{Th} only has coherences between states with n excitations. However, because the excitation number depends on both the TLS and the bosonic degree of freedom, it changes under partial transpose: A coherence between states with excitation number n can become a coherence between a state with excitation number $n-1$ and a state with

excitation number $n+1$ (e.g., for $n=1$, $|\uparrow, 0\rangle\langle\downarrow, 1|$ becomes $|\downarrow, 0\rangle\langle\uparrow, 1|$, where the first entry of the ket is the TLS state and the second the number of bosonic excitations). Since only states with excitation number n are populated in this thermal state, there is no population to “support” these partial transposed coherences (in the sense of maintaining the Cauchy-Schwarz inequality $\rho_{ii}^{\text{PT}}\rho_{jj}^{\text{PT}} \geq |\rho_{ij}^{\text{PT}}|^2$); this results in a Cauchy-Schwarz violation and a large $\mathcal{S}$. The only exception to the above discussion is when $|\lambda| \in (0, \lambda_0)$, where the thermal state has no coherence because the zero-excitation subspace is one dimensional, so $\mathcal{S} = 0$ and hence $\mathcal{N}$ should be 0 or small.

In contrast, as λ approaches λ_n , states within both the n and $n+1$ symmetry sectors are populated in the thermal state, and the populations of the ground states are halved compared to the $\lambda \in (\lambda_{n-1}, \lambda_n)$ case, leading to smaller coherences. There is still no population to support these coherences upon partial transposition, because the partial transposed coherences will involve states with $n-1$ or $n+2$ excitations, hence, a Cauchy-Schwarz violation still occurs. However, the smaller magnitude of the coherences means that the total violation $\mathcal{S}$ will be smaller. Consequently, one expects the negativity $\mathcal{N}$ and entanglement to also decrease at degeneracies.

These qualitative considerations based on the CSV condition can be confirmed by analytical zero-temperature calculations of $\mathcal{N}$ and $\mathcal{S}$ (see Sec. 1 of the Supplemental Material [37]). When $\lambda_{n-1} < |\lambda| < \lambda_n$, we find $\mathcal{S}(\rho_{\text{Th}}) = \frac{\lambda^2 n}{(\Delta-1)^2 + 4\lambda^2 n}$ in the $\{|\uparrow, n\rangle, |\downarrow, n\rangle\}$ product basis, and $\mathcal{N}(\rho_{\text{Th}}) = \sqrt{\mathcal{S}(\rho_{\text{Th}})}$, making the numerical correspondence between $\mathcal{S}$ and $\mathcal{N}$ precise in this case. In particular, $\mathcal{S}$ ($\mathcal{N}$) remains 0 until $|\lambda| \geq \lambda_0$, and then quickly asymptotes to 1/4 (1/2) with increasing $|\lambda|$. On the other hand, when $|\lambda| = \lambda_n$, the expressions for $\mathcal{S}(\rho_{\text{Th}})$ and $\mathcal{N}(\rho_{\text{Th}})$ are more complicated and no longer have a simple relation. However, the magnitudes of $\mathcal{S}$ and $\mathcal{N}$ are still qualitatively correlated, as both decrease relative to the nondegenerate case, with $\mathcal{S}$ now bounded by 1/8 and $\mathcal{N}$ by 1/3. All of these behaviors agree with the predictions of the CSV condition. This is further verified by numerical calculations (see Sec. 2 of the Supplemental Material [37]) of the thermal steady state and its $\sqrt{\mathcal{S}}$ and $\mathcal{N}$ at low but nonzero temperature; the results are shown in red in Fig. 1, with the dips at degeneracies broadened by the nonzero temperature. Altogether, the CSV condition connects the entanglement of the thermal state to its symmetry properties, revealing a link between the excitation number symmetry of the JCM and entanglement.

Given this connection between symmetry and entanglement, one would expect the QRM to display different entanglement behavior from the JCM because it only has $\mathbb{Z}_2$ symmetry. This difference can be predicted from the CSV condition alone, without any explicit computations. The H_{QRM} eigenstates can be labeled as even (+1 eigenstates of $P^{\mathbb{Z}_2}$) or odd (−1 eigenstates). Because the parity symmetry involves information about both the spin and boson subsystems, the partial transpose can move coherences between states with different symmetries, transforming certain coherences between even states (“even-even coherences”) into coherences between odd states (“odd-odd coherences”), and vice versa (for e.g., $|\uparrow, 0\rangle\langle\downarrow, 1| \rightarrow |\downarrow, 0\rangle\langle\uparrow, 1|$).

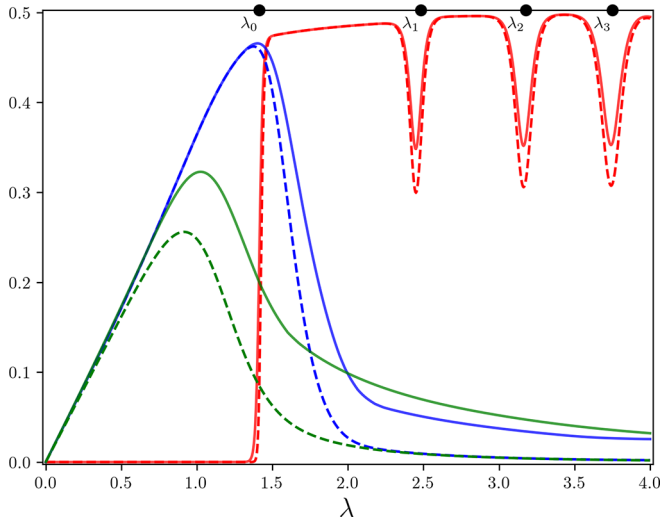


FIG. 1. Numerically calculated $\sqrt{S}$ (solid lines) and $\mathcal{N}$ (dashed lines) for the thermal states of H_{JCM} (red), H_{QRM} (blue), and H_ε for $\varepsilon = 0.1\Delta$ (green), with JCM degeneracies λ_n marked. For all calculations, $\Delta = 2$, $\beta = 90$.

We examine the dependence of entanglement of low-temperature QRM thermal states on coupling strength λ . When $\lambda \ll \Delta$, the TLS and the bosonic mode are only weakly coupled and the ground state $|G(\lambda)\rangle$ is dominated by $|\downarrow, 0\rangle$ weakly mixed with other even states. At low temperatures, the thermal state is approximately $|G(\lambda)\rangle\langle G(\lambda)|$, which has weak even-even coherences due to mixing, but no odd population. Upon partial transposing even-even coherences into odd-odd ones, there is no population to support them, so a weak Cauchy-Schwarz violation occurs and S will be small but nonzero.

In the intermediate-coupling regime $\lambda \approx \Delta$, the larger λ leads to stronger mixing of the ground state, resulting in larger even-even coherences. However, since Δ is still comparable to λ , the energy gap between the ground state (even) and the first excited state (odd) should remain large, so that only the ground state has a significant population at low temperatures. This combination of large even-even coherences and a negligible odd population ensures that partial transposition leads to a large S .

In the strong-coupling regime $\lambda \gg \Delta$, one can view $\frac{\Delta}{2}\sigma_z$ as a perturbation to $H_0 = \lambda\sigma_x(a + a^\dagger) + a^\dagger a$. By viewing the bosons as shifted harmonic oscillators, it is clear that all energy levels of H_0 are doubly degenerate, with one even state and one odd state per level. The $\frac{\Delta}{2}\sigma_z$ perturbation only slightly splits the degenerate ground state, so that both of the unperturbed ground states are significantly populated at low but nonzero temperature, resulting in large populations of both even and odd parity states. Although there are large even-even and odd-odd coherences due to the strong coupling λ , these coherences can be supported upon partial transposition through the large population of both types of parity states. Thus, surprisingly, S , and hence entanglement, is expected to be *suppressed* in the strong-coupling regime.

Altogether, from symmetry considerations alone, we expect S to depend nonmonotonically on the coupling strength λ , suggesting similar behavior for negativity. The

nonmonotonicity and correlation between S and $\mathcal{N}$ are confirmed numerically (with S computed in the $\{|\uparrow, n\rangle, |\downarrow, n\rangle\}$ product basis) in blue in Fig. 1. While the precise relation $\mathcal{N} = \sqrt{S}$ no longer holds, we see that $\mathcal{N}$ and $\sqrt{S}$ are still quantitatively similar. Furthermore, one can check that the magnitudes of the populations and coherences of the numerically calculated thermal states match the above qualitative predictions (see Sec. 3 of the Supplemental Material [37]).

From Fig. 1, one sees that the differing symmetries of the JCM and QRM are reflected through remarkably different entanglement behavior. Surprisingly, in the strong-coupling regime the entanglement in the QRM *decreases* with increasing coupling strength, unlike the JCM where it plateaus. Furthermore, for weak coupling, the QRM exhibits nonzero entanglement so long as the coupling is nonzero, whereas in the JCM, there is no entanglement until $|\lambda|$ passes a threshold. These disparate behaviors in the weak-coupling regime are remarkable because the only difference between the QRM and JCM is the presence of counterrotating terms, which one expects to have a negligible effect in the weak-coupling regime. As has been seen in studies of coupled TLS [38,39], the counterrotating terms have a significant effect on entanglement even in the weak-coupling regime because they alter the symmetry, and hence the coherence structure, of the system. The CSV condition provides the key insight that the counterintuitive differences in the thermal entanglement properties of the JCM and QRM, in both the weak- and strong-coupling regimes, are a consequence of the differing symmetries of the two models.

As additional evidence of the connection between symmetry and entanglement, we further reduce the symmetry by considering a modified QRM Hamiltonian $H_\varepsilon = \frac{\Delta}{2}\sigma_z + \varepsilon\sigma_x + \lambda\sigma_x(a + a^\dagger) + a^\dagger a$. According to the CSV condition, the buildup of negativity in the intermediate-coupling regime of the QRM is due to the $\mathbb{Z}_2$ symmetry forbidding odd population, which induces a large S . With the $\mathbb{Z}_2$ symmetry destroyed when $\varepsilon \neq 0$, this buildup of S and $\mathcal{N}$ should be suppressed. Additionally, as ε is increased, the maximum of S and $\mathcal{N}$ should shift to smaller λ due to the increased odd populations induced by mixing. Indeed, numerical calculations show that in the intermediate-coupling regime, both S and $\mathcal{N}$ are strongly suppressed in this modified system. The green curves in Fig. 1 show that even for a small perturbation of $\varepsilon = 0.1\Delta$, the maximal negativity is approximately halved and the peak occurs at a smaller λ ; further increasing ε further suppresses entanglement and shifts the peak to smaller λ (data not shown). The CSV condition allows for an intuitive understanding of how modifying a closed-system Hamiltonian will alter entanglement.

Rabi model with symmetry-respecting baths. There has been growing interest in open quantum systems where the bath also respects the symmetry of the system, leading to multiple steady states or a loss of ergodicity [40–45]. We briefly explore the use of the CSV condition in these scenarios.

Consider a QRM interacting with two independent bosonic baths via $H_{\text{sb}} = \gamma_e P_e T P_e \sum_k g_k (b_k^\dagger + b_k) + \gamma_o P_o T P_o \sum_l g_l (c_l^\dagger + c_l)$, where $P_e = (1 + P^{\mathbb{Z}_2})/2$ and $P_o = (1 - P^{\mathbb{Z}_2})/2$ are the even and odd projectors and $T = \sigma_x(a^\dagger + a)$. Here, $a^{(\dagger)}$ is the annihilation (creation)

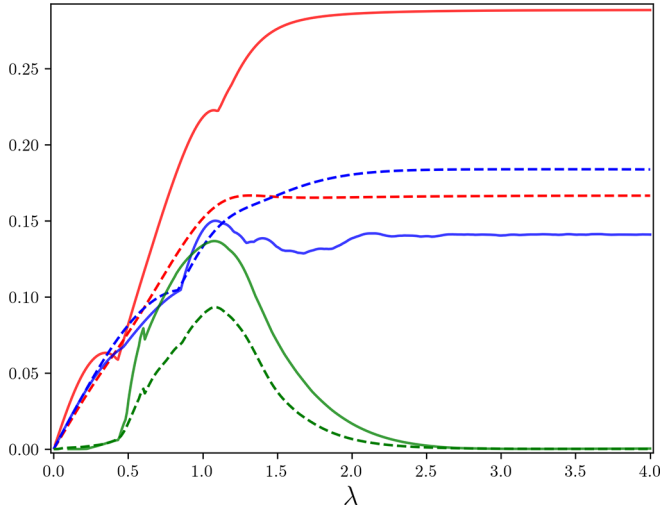


FIG. 2. Numerically calculated $\sqrt{S}$ (solid lines) and $\mathcal{N}$ (dashed lines) for various steady states for the symmetry-respecting bath. Red: $p_e = 2/3$, $p_o = 1/3$, $\beta_e = \beta_o = 90$. Blue: $p_e = p_o = 0.5$, $\beta_e = 90$, $\beta_o = 1$. Green: same as blue, but with $\varepsilon\sigma_x$ added to the Hamiltonian with $\varepsilon = 0.1\Delta$. For all calculations, $\Delta = 2$; Redfield calculations use $\gamma_e = \gamma_o = 1.4 \times 10^{-5}$ and spectral density $J(\omega) = \omega \exp(-\omega/\Delta)$ (details in Sec. 2 of the Supplemental Material [37]).

operator of the bosonic mode of the QRM, while $b^{(\dagger)}$ and $c^{(\dagger)}$ correspond to the modes of the “even bath” and “odd bath,” respectively. The projection operators ensure that the even bath thermalizes only the even subspace, while the odd bath thermalizes only the odd subspace.

If the even (odd) bath is held at inverse temperature β_e (β_o), the even and odd subspaces thermalize at inverse temperatures β_e and β_o , respectively, with the total populations p_e and p_o of each subspace unchanged from their initial values. Through the CSV condition, it is clear that negativity can be enhanced by tuning the populations p_e and p_o . For instance, if there is more population in the even subspace than in the odd one, there will be less odd population to support the larger even-even coherences, partially transposed into odd-odd ones. This should lead to a large buildup of S and $\mathcal{N}$, even in the strong-coupling regime. This is confirmed numerically in red in Fig. 2. Unlike in the original QRM, $\mathcal{N}$ and $\sqrt{S}$ both remain large even in the strong-coupling regime. The large entanglement that one intuitively expects to accompany strong coupling is manifest in the QRM if one of the parity subspaces is selectively populated.

The CSV condition also suggests that negativity can be enhanced via a temperature difference. Suppose that the temperature of the odd bath is increased, while the even bath is kept at low temperature. For large λ/Δ , the low-temperature even subspace has large even-even coherences because population is concentrated in the lowest-energy states, while the high-temperature odd subspace has its population spread across many excited states, with any individual state having a low population. These depopulated odd states can no longer support the partial transposed even-even coherences, leading to a larger S , and therefore a larger $\mathcal{N}$, in the strong-coupling regime. This is shown numerically in blue in Fig. 2. As

expected, S remains non-negligible in the strong-coupling regime, leading to an increased $\mathcal{N}$ compared to the original QRM.

Remarkably, this means that a higher temperature leads to *larger* negativity in the strong-coupling regime, despite the expectation that high temperatures destroy entanglement. Since this was rationalized through the connection between the CSV condition and $\mathbb{Z}_2$ symmetry, it is not surprising that it only occurs in the presence of the symmetry. Indeed, if one introduces the symmetry-breaking term $\varepsilon\sigma_x$ into the closed-system Hamiltonian, while retaining the parity-respecting system-bath interaction, one finds that the resulting nonequilibrium steady state (NESS) no longer displays enhanced negativity in the strong-coupling regime, as shown numerically in green in Fig. 2 for the NESS calculated using Redfield theory [19,46–48]. Not only is the increased S and $\mathcal{N}$ in the strong-coupling regime lost when comparing to the $\varepsilon = 0$ case, but also when compared to the green curve in Fig. 1, one sees that the negativity in the other regimes is significantly weakened compared to the thermal state of the QRM with $\varepsilon = 0.1\Delta$, in correspondence with the usual expectation that higher temperatures should inhibit entanglement. Once again, the CSV condition illuminates how the presence of the $\mathbb{Z}_2$ symmetry is critical to the negativity properties of the QRM.

The connection between symmetry and entanglement generalizes beyond the JCM and QRM. The same arguments suggest that any density operator whose populations and coherences are concentrated in one symmetry subspace will display high entanglement if a partial transpose can move the coherences to other symmetry subspaces. So long as a symmetry operator acts nontrivially (i.e., not as a multiple of the identity) on both subsystems, one generally expects a partial transpose to take some coherences out of any given symmetry eigenspace. Indeed, if no coherences are moved out of a symmetry eigenspace by partial transpose, and if the symmetry operator can be diagonalized in a product basis (so that it makes sense to talk about the symmetry label of product states), then that symmetry eigenspace must be of the form $U_i \otimes V_i$ for some subspaces U_i and V_i of the two subsystem Hilbert spaces. This is generally not the case for a symmetry operator acting nontrivially on both subsystems, though one notable exception is when a symmetry eigenspace is one dimensional, such as the $N = 0$ excitation subspace of the JCM that was associated with an unentangled thermal state. In general, a CSV symmetry analysis should focus on the coherences that move between the different symmetry subspaces under partial transpose.

Conclusion. We have introduced the use of the “Cauchy-Schwarz violation” condition, through which one detects entanglement in mixed states by looking for entries of the density operator such that $|\rho_{ij}^{\text{PT}}|^2 > \rho_{ii}\rho_{jj}$. The extent to which this occurs can be quantified by $S(\rho) = \sum_{i>j} \max\{|\rho_{ij}^{\text{PT}}|^2 - \rho_{ii}^{\text{PT}}\rho_{jj}^{\text{PT}}, 0\}$, and although nonzero S is only a sufficient condition for nonzero negativity, analytical and numerical examples demonstrate that in fact S has a close quantitative correspondence with the negativity.

The “local” nature of CSV gives it a simple physical interpretation as a local imbalance of population and coherence. This allows for intuitive understanding of entanglement behavior and enables connections between entanglement and

other physical properties of a system such as symmetries. This was exemplified by the symmetry analysis of the contrasting entanglement behaviors of the JCM and QRM, as well as the successful predictions of the impact of further symmetry modifications to the QRM on its entanglement. This suggests that the CSV condition could be a useful physical guide when engineering systems to maximize or suppress entanglement, particularly when symmetry can be used.

While the focus of this work has been on the steady states of simple models, the general principles should extend both to the time-dependent domain and to more realistic systems. In time-evolving open quantum systems, the CSV condition could be used to understand how the combination of population transport and the creation and destruction of coherences due to bath interactions leads to the dynamics of negativity. Furthermore, the close connection between symmetry and entanglement revealed by the CSV condition provides a way

to extend studies of model systems to more realistic settings: Even if a real system has different microscopic interactions than a model, it should show similar negativity so long as it obeys the same symmetries. On the other hand, one should not use models with more symmetries than the physical system of interest, because extra symmetries can drastically alter negativity properties, as seen from the comparison of the JCM and QRM.

Acknowledgments. This material is based upon U.S. Air Force Office of Scientific Research (AFOSR) under Grant No. FA9550-20-1-0354 and support from the Natural Sciences and Engineering Research Council of Canada (NSERC) and Centre for Quantum Information and Quantum Control (CQIQC).

Data availability. The data that support the findings of this article are openly available [49].

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