Negativity Hamiltonian: An Operator Characterization of Mixed-State Entanglement

Sara Murciano,[1,2] Vittorio Vitale,[1,3] Marcello Dalmonte,[1,3] and Pasquale Calabrese[1,2,3]
[1]SISSA, via Bonomea 265, 34136 Trieste, Italy
[2]INFN Sezione di Trieste, via Bonomea 265, 34136 Trieste, Italy
[3]The Abdus Salam International Center for Theoretical Physics, Strada Costiera 11, 34151 Trieste, Italy

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In the context of ground states of quantum many-body systems, the locality of entanglement between connected regions of space is directly tied to the locality of the corresponding entanglement Hamiltonian: the latter is dominated by local, few-body terms. In this work, we introduce the negativity Hamiltonian as the (non-Hermitian) effective Hamiltonian operator describing the logarithm of the partial transpose of a many-body system. This allows us to address the connection between entanglement and operator locality beyond the paradigm of bipartite pure systems. As a first step in this direction, we study the structure of the negativity Hamiltonian for fermionic conformal field theories and a free-fermion chain: in both cases, we show that the negativity Hamiltonian assumes a quasilocal functional form, that is captured by simple functional relations.

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Introduction.—Over the past two decades, entanglement has been a central concept in many branches of quantum physics ranging from quantum information [1,2] to condensed matter theory [3,4] and high-energy physics [5–9]. In particular, it has been successfully utilized to characterize quantum many-body systems both theoretically and experimentally [10–16]. The main object which enters in its quantification is the reduced density matrix (RDM). For a given state ρ, the RDM of a region A, ρ_A, is obtained by tracing ρ over the complement of A, B; that is,

$$\rho_A = \mathrm{Tr}_B \rho = \frac{e^{-H_A}}{Z_A}, \qquad Z_A = \mathrm{Tr} e^{-H_A}, \tag{1}$$

where the operator H_A is the entanglement (or modular) Hamiltonian (EH).

From a many-body viewpoint, the entanglement properties of pure states can be construed in a hierarchical manner. Firstly, there exists a characterization of its entanglement properties via entanglement entropies. Those are uniquely dependent on the spectrum of H_A—also known as entanglement spectrum. Secondly, it is possible to characterize the properties of the RDM directly at the operator level, via the full characterization of the EH—a paradigmatic example being the Li-Haldane conjecture in the context of topological matter [17].

The EH fully characterizes the "local" properties of entanglement in a many-body system; that is, it allows us to understand whether the RDM can be interpreted as the exponential of a local operator composed solely of few-body local terms. In the context of quantum field theory, this principle of locality is an established pillar: the Bisognano-Wichmann (BW) theorem [18,19]. Such locality is at the heart of several physical phenomena—from topological order to the nature of area laws in gapped systems—and is the key element at the basis of theory and experiments aimed at large-scale reconstructions of the RDM [20–22]. However, it is presently unknown whether it is possible to associate locality and entanglement in a similar way for the case of mixed-state entanglement, that encompasses a variety of scenarios of key experimental and theoretical relevance, from mixed states to correlations between partitions in pure states.

In this work, we introduce and investigate the negativity Hamiltonian (NH), an operator that allows us to cast the relation between locality and entanglement (in particular, that related to Peres-Horodecki criterion) for general mixed states. Our work is directly motivated by a series of recent results that have emphasized the importance of the entanglement negativity in a variety of settings, including harmonic oscillator chains [23–29], quantum spin models [30–38], free fermionic systems [39–44], $(1+1)D$ conformal and integrable field theories [45–55], out-of-equilibrium settings [56–64], and topological order [65–70]. Importantly, the negativity is directly linked to the partial transpose $\rho_A^{T_1}$ of the RDM, and, as such, does lend itself naturally to an interpretation based on statistical mechanics. For the case of a subpartition of $A = A_1 \cup A_2$, we define the *negativity Hamiltonian* $\mathcal{N}_A$ as

$$\rho_A^{T_1} = Z_A^{-1} e^{-\mathcal{N}_A}. \tag{2}$$

Clearly $\mathcal{N}_A$ is non-Hermitian because negative eigenvalues of $\rho_A^{T_1}$ are the signature of mixed-state entanglement. Nevertheless, it is still natural to wonder about the locality

properties of $\mathcal{N}_A$ and about the location of its eigenvalues in the complex plane.

After discussing the definition of $\mathcal{N}_A$ for both bosonic (spin) and fermionic systems, we unveil the operator structure of $\mathcal{N}_A$ for two relevant cases: $(1+1)$d fermionic conformal field theory and a tight-binding model of spinless fermions on a chain. Both cases show a characteristic quasilocal (in a sense to be specified below) structure—a first demonstration of the relation between entanglement and locality at the operator level beyond the case of complementary partitions. On top of its conceptual relevance, and similarly to what has been discussed in the context of pure states for the case of local EHs, this fact enables some immediate consequences: (i) interpreting the negativity spectrum, i.e., the analog of the pure-state entanglement spectrum for mixed states [38,50], (ii) simulating this object in nowadays available quantum platforms [10], and (iii) applying well-established statistical mechanics tools such as tensor networks [71,72] and quantum Monte Carlo techniques [73] to access the entire partial transpose $\rho_A^{T_1}$.

Partial transpose.—To introduce the concept of the negativity Hamiltonian, the first step is to discuss the partial transpose for bosonic and fermionic systems. Let us start by considering a bosonic system $A = A_1 \cup A_2$ described by

$$\rho_A = \sum_{i,j,k,l} \langle e_i^{A_1}, e_j^{A_2}|\rho_A|e_k^{A_1}, e_l^{A_2}\rangle |e_i^{A_1}, e_j^{A_2}\rangle\langle e_k^{A_1}, e_l^{A_2}|, \quad (3)$$

where $|e_i^{A_1}\rangle, |e_j^{A_2}\rangle$ denote orthonormal bases in the Hilbert spaces $\mathcal{H}_{A_1}$ and $\mathcal{H}_{A_2}$ corresponding to subsystems A_1 and A_2. The partial transpose of the reduced density matrix $\rho_A^{T_1}$ with respect to the system A_1 is defined performing a standard transposition in $\mathcal{H}_{A_1}$, i.e., exchanging the matrix elements in A_1, $\rho_A^{T_1} = (T_{A_1} \otimes \mathbb{1}_{A_2})\rho_A$. The presence of negative eigenvalues of $\rho_A^{T_1}$ is a signature of mixed-state entanglement [74], which can be quantified by the logarithmic negativity $\mathcal{E} = \log \mathrm{Tr}|\rho_A^{T_1}|$ [75,76].

The partial transposition also has an interpretation in terms of a time-reversal transformation or mirror reflection in phase space [77]. Namely, considering the one-to-one correspondence between density matrices and Wigner distribution functions $W(q,p)$, then $\rho_A \to \rho_A^T \Leftrightarrow W(q,p) \to W(q,-p)$. This can be conveniently observed starting from a bosonic density matrix written in a coherent state basis, since time-reversal transformation ($\mathcal{T}$) can be identified with the complex conjugation [39]. Taking $|\alpha\rangle$, a bosonic coherent state, one has

$$(|\alpha\rangle\langle\alpha^*|) \xrightarrow{\mathcal{T}} |\alpha^*\rangle\langle\alpha| = (|\alpha\rangle\langle\alpha^*|)^T. \quad (4)$$

In the case of fermionic systems, the equivalence above does not hold and the definition of partial transposition differs when looking at the density matrix or at the Wigner distribution function. In a coherent state basis the RDM reads [39,44,78,79]

$$\rho_A = \frac{1}{Z}\int d[\xi]d[\bar{\xi}]e^{-\sum_j \bar{\xi}_j\xi_j}\langle\{\xi_j\}|\rho_A|\{\bar{\xi}_j\}\rangle|\{\xi_j\}\rangle\langle\{\bar{\xi}_j\}|. \quad (5)$$

Here $\xi, \bar{\xi}$ are Grassman variables and $|\xi\rangle = e^{-\xi a^\dagger}|0\rangle$, $|\bar{\xi}\rangle = \langle 0|e^{-a^\dagger\bar{\xi}}$ are the related fermionic coherent states. The partial time reversal, analog of Eq. (4), is [39]

$$|\xi\rangle\langle\bar{\xi}| \xrightarrow{\mathcal{T}} |i\bar{\xi}\rangle\langle i\xi|. \quad (6)$$

The partial time reversal $\rho_A^{R_1}$, obtained by acting with Eq. (6) in Eq. (5) only in A_1, provides the fermionic negativity as $\mathcal{E} = \log \mathrm{Tr}|\rho_A^{R_1}|$, although its spectrum is not real in general [40]. To have a more transparent interpretation of the fermionic negativity, an alternative partial transpose, called twisted fermionic partial transpose, has been defined as [40]

$$\rho_A^{\tilde{R}_1} = \rho_A^{R_1}(-1)^{F_{A_1}}, \quad (7)$$

where $F_{A_1} = \sum_{j\in A_1} n_j$ is the number of fermions in the subsystem A_1. This new object has only real eigenvalues and the logarithmic negativity,

$$\mathcal{E} = \log \mathrm{Tr}|\rho_A^{\tilde{R}_1}|, \quad (8)$$

is a measure of the negativeness of the eigenvalues, exactly as for the bosonic partial transpose. We define the negativity Hamiltonian related to $\rho_A^{R_1}$ as $\mathcal{N}_A$ and the one related to $\rho_A^{\tilde{R}_1}$ as $\tilde{\mathcal{N}}_A$.

Bisognano-Wichmann theorem.—The BW theorem gives a general structure for the entanglement Hamiltonian of the ground state of a relativistic invariant quantum field theory with Hamiltonian density $H(\mathbf{x})$, when considering a bipartition between two half-spaces of an infinite system. In formulas, considering a d-dimensional system, $\mathbf{x} = \{x_1, \ldots, x_d\}$ and a partition $A = \{\mathbf{x}|x_1 > 0\}$, the EH of the ground state is $H_A = 2\pi \int_{\mathbf{x}\in A} d\mathbf{x} x_1 H(\mathbf{x}) + c$, where c is a normalization constant. This result does not depend on the dimensionality of the system or on any *a priori* knowledge of the ground state and can be applied to a large variety of systems and quantum phases. For conformal invariant theories, the BW theorem is easily generalized to some different geometries by conformal mappings [80–83]. This equivalence does not hold when A is the union of two disjoint intervals, but, nevertheless, the EH for this geometry is known for $(1+1)$-dimensional free Dirac fermions [84]. In this case, it is possible to identify a local part in the entanglement Hamiltonian proportional to the energy density and a quasilocal part quadratic in the fermionic field. We will make explicit use of this example

in the following. We will also check our analytical prediction against lattice simulations. In fact, the BW theorem can be used to construct approximate entanglement Hamiltonians for lattice models. This has been extensively investigated both for one- and two-dimensional models and it has been shown that the approximation provided by BW theorem allows us to build entanglement Hamiltonians that encode all the relevant entanglement properties of the ground states [85–87].

Negativity Hamiltonian and its quasilocal structure.— To build the negativity Hamiltonian, we should first recall the path integral construction of the (bosonic) partial transpose [46,47]. The partial transposition corresponds to the exchange of row and column indices in A_1 which naturally leads to a space inversion within A_1. On a fundamental level, this fact can be deduced from *CPT* theorem. Indeed, the partial transposition is equivalent to a partial time reversal that, by *CPT*, is the same as a parity operation in the world sheet combined with a charge conjugation. This second construction holds true also for $\rho_A^{R_1}$ in fermionic systems.

Therefore, starting from the entanglement Hamiltonian for two disjoint intervals and doing a spatial inversion of the interval $A_1 = [a_1, b_1]$, one obtains the partial time reversal of the density matrix. Although this procedure is fully general, the entanglement Hamiltonians of disjoint intervals are known only in few cases [84,88–94]. In particular, starting from the EH for the massless real (Majorana) fermion $\Psi(x)$ [84], $\Psi(x) = \begin{pmatrix} \psi_1(x) \\ \psi_2(x) \end{pmatrix}$, and performing this inversion, we get after simple algebra [95]:

$$\begin{aligned} \mathcal{N}_A &= \mathcal{N}_{A,\mathrm{loc}} + i\mathcal{N}_{A,\mathrm{qloc}}, \\ \mathcal{N}_{A,\mathrm{loc}} &= 2\pi \int_A \beta^R_{\mathrm{loc}}(x) T_{tt}(0,x)dx, \\ \mathcal{N}_{A,\mathrm{qloc}} &= 2\pi \int_A \beta^R_{\mathrm{qloc}}(x) T_{\mathrm{qloc}}(x, \bar{x}^R(x))dx, \end{aligned} \tag{9}$$

where

$$\beta^R_{\mathrm{loc}}(x) = \frac{1}{w^{R\prime}(x)}, \qquad \beta^R_{\mathrm{q-loc}}(x) = \frac{\beta^R_{\mathrm{loc}}(\bar{x}^R(x))}{x - \bar{x}^R(x)}, \tag{10}$$

with

$$\begin{aligned} w^R(x) &= \log\left[-\frac{(x-b_1)(x-a_2)}{(x-a_1)(x-b_2)}\right], \\ \bar{x}^R(x) &= \frac{(a_1b_2 - b_1a_2)x + (a_1+b_2)b_1a_2 - (b_1+a_2)a_1b_2}{(a_1 - b_1 + b_2 - a_2)x + b_1a_2 - a_1b_2}. \end{aligned} \tag{11}$$

Here $T_{tt}(0,x)$ is the energy density operator of the theory while $T_{\mathrm{qloc}}(x,\bar{x})$ is a bilinear of the real fermionic fields, with $x \in A_1$ and $\bar{x} \in A_2$ (and vice versa); i.e.,

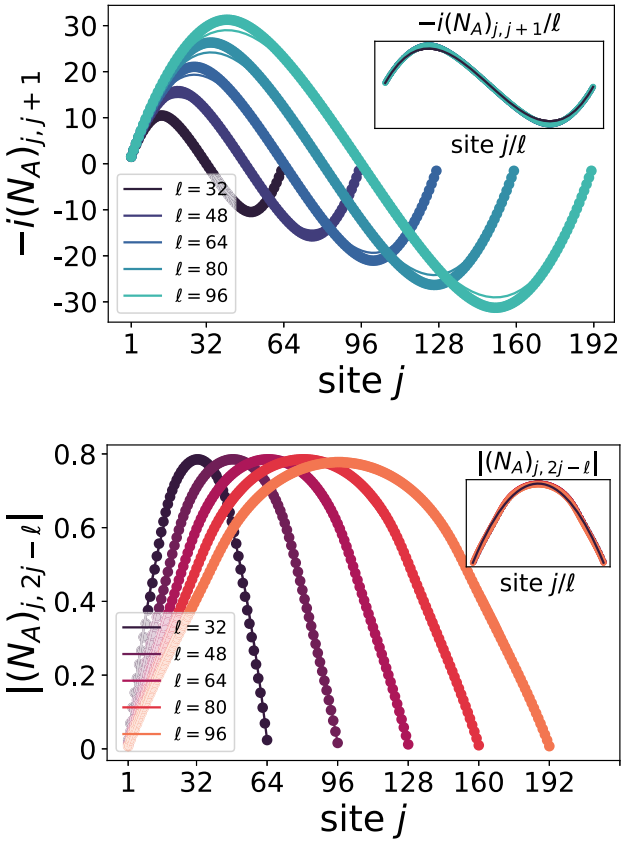

FIG. 1. Benchmark of the analytical prediction for the negativity Hamiltonian of a real fermion. We consider $A_1 = [1,\ell], A_2 = [\ell+1, 2\ell]$ embedded in the infinite line. The symbols correspond to numerical data, while the solid lines correspond to the discretized form of Eq. (9). Upper panel: $N_{A,\mathrm{loc}}$. Lower panel: $|N_{A,\mathrm{qloc}}|$. Insets: data collapse

$$T_{\mathrm{qloc}}(x,y) \equiv i{:}(\psi_1(x)\psi_1(y) - \psi_2(x)\psi_2(y)){:}. \tag{12}$$

The structure of Eq. (9) is very suggestive: it consists of a local term proportional to the energy density and an additional nonlocal part given by a quadratic expression in the fermionic field. The latter, however, has a mild nonlocality: each point $x \in A_1$ is coupled to only a specific $y = \bar{x}^R \in A_2$ (that is a consequence of the mirror symmetry for equal intervals). Thus, following Ref. [84], we refer to $\mathcal{N}_{A,\mathrm{qloc}}$ as a quasilocal operator. Its existence is the reason for the imaginary components in the spectrum of $\mathcal{N}_A$, which is one characteristic treat of $\rho_A^{R_1}$. The shape of $|\mathcal{N}_{A,\mathrm{qloc}}|$ (see also Fig. 1) is compatible with the results of the negativity contour [42] suggesting that the largest contribution to the negativity comes from the boundary region between A_1 and A_2.

To test the validity of Eq. (9), we consider a lattice discretization of the Hamiltonian of free real fermions. Because of the Gaussianity of $\rho_A^{R_1}$ [39], the numerical evaluation of the negativity Hamiltonian amounts to compute the single particle operator N_A defined as

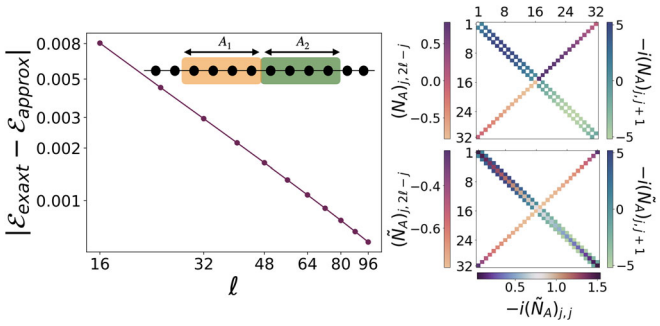

FIG. 2. Summary of our results for adjacent intervals of equal length ℓ on the infinite line for lattice free-fermions (geometry in the inset). The one-particle negativity Hamiltonians N_A and $\tilde{N}_A$ are dominated by quasilocal terms appearing close to the diagonal and on the antidiagonal (see the right-hand panels for $\ell = 8$). Left-hand panel: comparison of the exact logarithmic negativity with the approximate one coming from field theoretical $\tilde{N}_A$; see text.

$\mathcal{N}_A = \sum_{ij}(N_A)_{i,j}\psi_j\psi_i$, related to the covariance matrix [101,102]. We focus on two equal adjacent intervals $A = A_1 \cup A_2$ made up of ℓ sites labeled by $1 \le j \le 2\ell$. In this case, the point $\bar{x}^R$ in Eq. (11) is just $\bar{x}^R = 2\ell - x$ and so the quasilocal term lies entirely on the antidiagonal. As a consequence, in Fig. 1 we show only the subdiagonal $(N_A)_{j,j+1}$ [a similar behavior can be found for $(N_A)_{j+1,j}$] and the antidiagonal $(N_A)_{j,2\ell-j}$ which correspond, respectively, to the local and to the quasilocal parts of N_A. The agreement between lattice exact and field-theoretical discretized N_A is remarkable over the all parameter regime, and even for modest system sizes. Small discrepancies up to a few percent are present far from the boundaries: those have very little effect on the negativity, as they affect only very small (in absolute value) eigenvalues of the partial transpose. We verified that the other matrix elements of N_A are negligible, in the sense that they are subleading as $\ell \to \infty$ (in the same sense as subleading terms in the EH are negligible; see Refs. [85–87,103–107]).

We have also studied the structure of negativity Hamiltonian $\tilde{\mathcal{N}}_A$ for two adjacent intervals of equal length, $\ell_1 = \ell_2 = \ell$. We remind that $\rho_A^{\tilde{R}_1} = Z_A^{-1}e^{-\tilde{\mathcal{N}}}$, where $\rho_A^{\tilde{R}_1}$ is defined in Eq. (7). The advantage in the analysis of this operator is that it is Hermitian, so the logarithmic negativity recovers its original meaning of measure of the negativeness of the eigenvalues, as we are going to show by discussing the spectrum of this operator. Although we did not manage to derive its form explicitly, we provide a conjecture that very accurately matches numerical data on the lattice. It reads $\tilde{\mathcal{N}}_A = \tilde{\mathcal{N}}_{A,\mathrm{diag}} + \tilde{\mathcal{N}}_{A,\mathrm{loc}} + \tilde{\mathcal{N}}_{A,\mathrm{qloc}}$, with

$$\begin{aligned}
\tilde{\mathcal{N}}_{A,\mathrm{diag}} &= 2\pi i \int_A \tilde{\beta}_{\mathrm{diag}}(x)dx, \\
\tilde{\mathcal{N}}_{A,\mathrm{loc}} &= 2\pi \int_A \tilde{\beta}_{\mathrm{loc}}(x)dx T_{tt}(0,x), \\
\tilde{\mathcal{N}}_{A,\mathrm{qloc}} &= 2\pi \int_A \tilde{\beta}_{\mathrm{q-loc}}(x) T_{\mathrm{qloc}}(x,\bar{x}^R)dx,
\end{aligned} \tag{13}$$

where

$$\begin{aligned}
\tilde{\beta}_{\mathrm{diag}}(x) &= \frac{1}{2} - \frac{x}{8\ell}, \\
\tilde{\beta}_{\mathrm{loc}} &= -\frac{x(8\ell^2 - 6\ell x + x^2)}{8\ell^2}, \\
\tilde{\beta}_{\mathrm{qloc}}(x) &= 4\left(\frac{x - 2\ell - \frac{1}{2}}{4\ell}\right)^4 + \frac{1}{2}\left(\frac{x - 2\ell - \frac{1}{2}}{4\ell}\right)^2 - \frac{1}{2}.
\end{aligned} \tag{14}$$

Let us observe that by choosing $a_1 = 0, b_1 = a_2 = \ell, b_2 = 2\ell$, $\tilde{\mathcal{N}}_{A,\mathrm{loc}}$ and $\mathcal{N}_{A,\mathrm{loc}}$ coincide, while $\tilde{\mathcal{N}}_{A,\mathrm{nonloc}}$ and $\mathcal{N}_{A,\mathrm{nonloc}}$ are different because the former is a quartic function of x, while the latter is quadratic. As a nontrivial test for the accuracy of this conjecture, we verified that it provides a logarithmic negativity that, as ℓ increases, approaches the exact numerical value (see Fig. 2). We also benchmarked the analytical predictions from Eq. (13) for free real fermions on the lattice, as shown in Fig. 3, for the one-particle NH, i.e., $\tilde{\mathcal{N}}_A = \sum_{ij}(\tilde{N}_A)_{i,j}\psi_j\psi_i$. Remarkably, the formulas above are in good agreement with simulations and, as already observed, the small discrepancies do not affect sizably the logarithmic negativity approximation. The inset

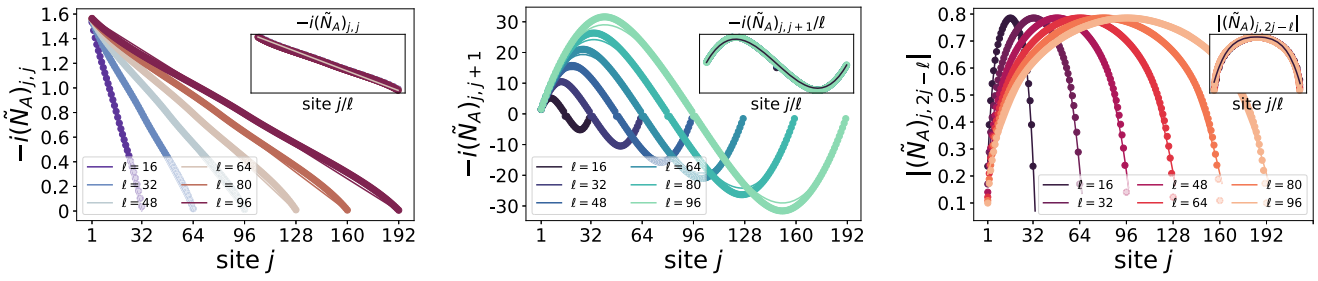

FIG. 3. Benchmark of the analytic prediction for the negativity Hamiltonian $\tilde{N}_A$. The symbols correspond to numerical data, while the solid lines correspond to the discretized form of Eq. (13) for two adjacent intervals of length ℓ. From left to right: comparison $\tilde{N}_{A,\mathrm{loc}}$, $\tilde{N}_{A,\mathrm{qloc-loc}}$, and $\tilde{N}_{A,\mathrm{qloc}}$ with exact lattice simulations. Insets: data collapse

illustrates how results from different partition sizes collapse onto a single functional form, signaling scale invariance.

A final comment concerns the spectrum of $\tilde{N}_A$: it consists of two parts, $\{\lambda_j + i\pi\}, \lambda_j \in \mathbb{R}$ for $j = 1, \ldots, 2\ell$ and $\{\lambda_j\}, \lambda_j \in \mathbb{R}$ for $j = 2\ell + 1, \ldots, 4\ell$. By simple exponentiation, we get the eigenvalues of $\rho_A^{\tilde{R}_1}$; see Supplemental Material [95]. We can then trace back the appearance of negative eigenvalues in the spectrum of $\rho_A^{\tilde{R}_1}$ (and, as a consequence, of a nonzero negativity) to the presence of the factors $i\pi$ in $\tilde{N}_A$.

Other tests of the analytic formulas for the negativity Hamiltonian N_A, including different and disjoint intervals, are reported in the Supplemental Material [95].

Discussion and outlook.—In this work we initiated the study of the negativity Hamiltonian in many-body quantum systems. Although our field-theoretical construction in terms of the EH of disjoint intervals is very general, its applicability relies crucially on the exact knowledge of the latter, that is not always available. We hope that this work will spark further studies on disjoint intervals's EH and, at the same time, the search for alternative constructions of N_A. Furthermore, we stress that the knowledge of this operator encodes the entire information content about the entanglement in the mixed states. This is remarkable with respect to the scalar quantities used to compute the entanglement (e.g., the negativity), which do not allow us to reconstruct the whole partial transpose reduced density matrix. We expect that the quasilocal structure of the negativity Hamiltonian can be generalized to other contexts, at least for free-fermions, such as a single interval in an infinite system at finite temperature [83], or two disjoint intervals in the presence of a pointlike defect [91]. At present, it is unclear whether this quasilocal structure survives to finite interaction strengths and in higher dimensions.

Having established an explicit approximate functional form for the negativity Hamiltonian that is quasilocal opens up several possible applications. First, one could design experiments aimed at a direct realization of N_A: since the corresponding operators have simple functional form, this could be done by combining local tuning with tailor-engineered long-distance couplings similarly to what has already been proposed in the context of quantum chemistry simulations [108]. Second, the local structure of N_A paves the way for a direct reconstruction of partial transposes in experiments, utilizing, e.g., Hamiltonian reconstruction methods that have already been combined with the BW theorem [21]. Both of these applications would allow a direct measurement of the negativity spectrum, something that is presently unachievable by any method other than full state tomography. Third, it may be possible to design efficient classical or hybrid classical-quantum algorithms for the *ab initio* determination of N_A, similarly to what has been done for the EH following a BW inspired ansatz [20,22,109]. Having an explicit functional form could enable computations that are then not available otherwise—one example being quantum Monte Carlo algorithms aimed at computing the negativity utilizing metadynamics, similarly to what has been done in the context of the EH [110].

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S. M. and V. V. contributed equally to this work.

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