

Lieb-Schultz-Mattis Theorem for Open Quantum Systems

1. Lieb-Schultz-Mattis Theorem in Open Quantum Systems


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2. Reviving the Lieb–Schultz–Mattis Theorem in Open Quantum Systems

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Recommended with a Commentary by Daniel Arovas , University of California, San Diego

The Lieb-Schultz-Mattis (LSM) theorem [1] is among the most consequential results in the theory of quantum magnetism. It guarantees that for an antiferromagnetic quantum spin- S chain whose Hamiltonian H is short-ranged, translationally invariant, and has a global $U(1)$ spin symmetry, the (singlet) ground state is either gapless or doubly degenerate in the thermodynamic limit $L \rightarrow \infty$ if S is a half-odd integer. The original (1963) proof utilizes the spin twist operator, $U = \exp(2\pi i \sum_{j=1}^L j S_j^z / L)$. One then has $U^\dagger S_n^\pm U = \exp(\mp 2\pi i n / L) S_n^\pm$, as well as $U^\dagger t U = e^{-2\pi i S} t$, where t is the lattice translation operator. If $|\Psi_0\rangle$ is a ground state of H , and we define $|\Psi_1\rangle = U |\Psi_0\rangle$, then since under the twist $S_n^+ S_{n+1}^- \rightarrow e^{2\pi i / L} S_n^+ S_{n+1}^-$, to lowest nontrivial order in L^{-1} and assuming reflection symmetry of H ,

$$E_1 = \langle \Psi_1 | H | \Psi_1 \rangle = \langle \Psi_0 | H | \Psi_0 \rangle + \frac{2\pi^2}{L^2} \langle \Psi_0 | H_\perp^{\text{loc}} | \Psi_0 \rangle = E_0 + \mathcal{O}(L^{-1}) \quad , \quad (1)$$

where H_\perp^{loc} is local. Furthermore, if $t |\Psi_0\rangle = e^{iK_0} |\Psi_0\rangle$, then $t |\Psi_1\rangle = e^{iK_1} |\Psi_1\rangle$ with $K_1 = K_0 - 2\pi S$. Thus, if $S \in \mathbb{Z} + \frac{1}{2}$, we have $\langle \Psi_1 | \Psi_0 \rangle = 0$ because $|\Psi_0\rangle$ and $|\Psi_1\rangle$ have inequivalent crystal momenta. Ta da!

A straightforward generalization to any higher dimension $d > 1$ fails because the bound one obtains is $E_1 \leq E_0 + \mathcal{O}(L^{d-2})$. However, Oshikawa's flux-threading argument charts a way forward. Place the system on a d -torus, and adiabatically thread a $U(1)$ flux ϕ through one of its cycles. This may be done in a translationally invariant way¹ so that

¹One replaces $S_r^+ S_{r'}^- \rightarrow S_r^+ S_{r'}^- \exp \left\{ i \int_r^{r'} d\ell \cdot \mathbf{A}_\phi(\ell) \right\}$, where $\mathbf{A}_\phi(\ell) = \phi \hat{\mathbf{e}} / L$ is the vector potential of a geometric flux tube threading a cycle of the d -torus in the $\hat{\mathbf{e}}$ direction.

$[H(\phi), t] = 0$ and crystal momentum is preserved throughout the adiabatic flux insertion process. If $|\Psi_0(\phi)\rangle$ is an adiabatic ground state of $H(\phi)$, one can ‘pull back’ from the Hilbert space of $H(2\pi)$ to that of $H(0)$ via the large gauge transformation U^\dagger using the LSM spin twist operator, defining $|\Psi_1\rangle = U^\dagger |\Psi_0(2\pi)\rangle$. One then finds $\mathbf{K}_1 - \mathbf{K}_0 = 2\pi N_\perp S \hat{\mathbf{e}}$, where $\hat{\mathbf{e}}$ is the unit vector in the direction of the flux insertion, and N_\perp is the number of lattice sites in the hyperplane perpendicular to $\hat{\mathbf{e}}$. If N_\perp is odd, then LSM follows for $S \in \mathbb{Z} + \frac{1}{2}$. One assumes (unproven) that this holds for any system dimensions in the thermodynamic limit².

In recent years there has been a great deal of activity in studying open quantum systems, such as in cases where a quantum system is in contact with a bath with which it may exchange energy, particle number, magnetization, *etc.* In this context, the system is described not by a wavefunction, but rather by a density matrix. Is there a generalization of LSM to open quantum systems?

Kawabata, Sohal, and Ryu (KSR) [2] considered quantum systems governed by the GKLS master equation [4],

$$\frac{d\varrho}{dt} = \mathcal{L}\varrho = -i[H, \varrho] + \sum_n \left(L_n \varrho L_n^\dagger - \frac{1}{2} L_n^\dagger L_n \varrho - \frac{1}{2} \varrho L_n^\dagger L_n \right) \quad , \quad (2)$$

where $\varrho(t)$ is the reduced density matrix of the system, H is the Hamiltonian, and the $\{L_n\}$ are ‘jump operators’ which embody the effects of the environment. The quantum Liouvillean superoperator \mathcal{L} generates a map $\mathcal{C}_t = \exp(\mathcal{L}t)$ which acts on density matrices, such that $\mathcal{C}_t \varrho(0) = \varrho(t)$. The map \mathcal{C}_t is (i) linear, (ii) trace-preserving, (iii) hermiticity-preserving, and (iv) completely positive³. Trace preservation entails that there is at least one (and possibly more, under nongeneric circumstances [5]) nonequilibrium steady state (NESS) ϱ_0 satisfying $\mathcal{L}\varrho_0 = 0$. In any basis, the density matrix $\varrho = \sum_{\alpha,\beta} \varrho_{\alpha\beta} |\alpha\rangle\langle\beta|$ may be expressed as a vector $|\varrho\rangle = \sum_{\alpha,\beta} \varrho_{\alpha\beta} |\alpha\rangle \otimes |\beta\rangle$, a manipulation known as the Choi-Jamiołkowski isomorphism. Eqn. 2 may then be recast as a non-Hermitian Schrödinger equation, $i d|\varrho\rangle/dt = \mathcal{H}|\varrho\rangle$, with \mathcal{H} acting on a doubled Hilbert space, *viz.*

$$\mathcal{H} = H \otimes I - I \otimes H + i \sum_n \left(L_n \otimes L_n^* - \frac{1}{2} L_n^\dagger L_n \otimes I - I \otimes \frac{1}{2} L_n^\dagger L_n \right) \quad , \quad (3)$$

where I is the identity⁴. The eigenvalues E_a of \mathcal{H} all satisfy $\gamma_a = -\text{Im}(E_a) \geq 0$, where $\{\gamma_a\}$ is the spectrum of relaxation rates. Any NESS has $E_a = 0$.

One may now define two types of symmetries [7]. A *strong symmetry* is one which commutes with H and all the L_n , whereas a *weak symmetry* commutes only with \mathcal{L} as a whole. KSR consider a system with translational invariance and strong U(1) symmetries

²More generally, Oshikawa showed that if the U(1) charge per unit cell is $\nu = p/q$ with p and q relatively prime, then a unique gapped ground state cannot exist when $\nu N_\perp \neq \mathbb{Z}$. To elicit a gap then requires a breaking of translational symmetry in which the unit cell is q -fold enlarged. For quantum spins, the local U(1) charge is $n_j = S_j^z + S$.

³A map \mathcal{C} is completely positive if $(\mathcal{C}\varrho) \otimes \omega$ is positive whenever $\varrho \otimes \omega$ is positive. Positivity means that $\langle \Psi | \varrho | \Psi \rangle \geq 0$ for all $|\Psi\rangle$. An example of a linear map which preserves trace and hermiticity yet which is not completely positive is matrix transposition.

⁴There is no new physics revealed by expressing Eqn. 2 in this way, but it perhaps provides a more familiar setting, as well as entailing some notational conveniences.

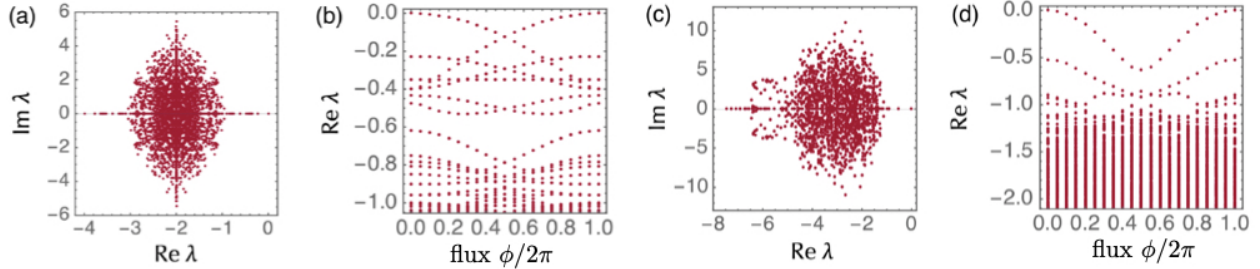


Figure 1: Fig. 1 from Ref. [2]. Eigenvalues λ of the dissipative XXZ quantum Liouvillian $\mathcal{L}(\phi)$ in the Heisenberg limit $\Delta = \eta = 1$ and total filling $\nu = \frac{1}{2}$, *i.e.* $S_{\text{tot}}^z = 0$. ($E = i\lambda$ are the eigenvalues of \mathcal{H} in Eqn. 3; the relaxation rates are $\gamma = -\text{Re } \lambda \geq 0$.) (a,b) $S = \frac{1}{2}$, $L = 8$. (c,d) $S = 1$, $L = 5$. In both cases the $U(1)$ flux is adiabatically inserted in the first (+) Hilbert space. For all flux ϕ there is an infinite temperature NESS with $\lambda = 0$ (not shown in panels b and d).

\mathcal{U}_{\pm} , where $\mathcal{U}_{+} = U_{+} \otimes I$ and $\mathcal{U}_{-} = I \otimes U_{-}$. (Translational invariance is a weak symmetry.) The unitary symmetries guarantee conserved charges N_{\pm} in the two Hilbert spaces, where $N_{\pm} = \sum_j (S_{j,\pm}^z + S)$. Assuming $N_{+} = N_{-}$, they show that if $\nu \equiv N_{\pm}/V$ is not an integer (V is the total number of spins), then \mathcal{L} is either gapless or exhibits degenerate NESS. The proof directly follows Oshikawa's derivation of LSM. Results for the XXZ Hamiltonian

$$H = \sum_{n=1}^L \left(S_n^x S_{n+1}^x + S_n^y S_{n+1}^y + \Delta S_n^z S_{n+1}^z \right) \quad (4)$$

with jump operators $L_n = \sqrt{\eta} S_n^z$ are shown in Fig. 1. A $U(1)$ flux ϕ_{\pm} may be inserted in either Hilbert space in a translationally-invariant way with periodic boundary conditions (see footnote 1 above), or by imposing twisted boundary conditions $S_{n+L,\pm}^{\pm} = \exp(i\phi_{\pm}) S_{n,\pm}^{\pm}$, which breaks translational invariance. Because all jump operators are Hermitian, it is easy to see that the infinite temperature state $\varrho_0 = 2^{-L} I$ is a NESS for any ϕ . Panels (a,b) show results for a dissipative $S = \frac{1}{2}$ chain, while panels (c,d) correspond to $S = 1$. Each dot corresponds to an eigenvalue of $\mathcal{L}(\phi) = -i\mathcal{H}(\phi)$. For $S = \frac{1}{2}$, the spectral flow in panel (b) shows crossings at the time-reversal symmetric value $\phi = \pi$, whereas for $S = 1$ panel (d) there are no such crossings. The numerics are for small system sizes ($L = 8$ and $L = 5$), and presumably as $L \rightarrow \infty$ this flow results in a dense set of states in the vicinity of $\lambda = 0$ for $S = \frac{1}{2}$, and that this is not the case for $S = 1$. Such a scenario would be consistent with KSR's version of LSM. Much more is explored in the body of KSR as well as in the supplemental material, but on to paper #2.

In Ref. [3], Zhou *et al.* approach the issue from the perspective of the entanglement Hamiltonian $K \equiv -\ln \varrho_s$ [8], where $\varrho_s = \text{Tr}_b(|\Psi_0\rangle\langle\Psi_0|)$ is the reduced density matrix of a system *explicitly* coupled to an environmental bath, rather than obtained as a NESS from GKLS dynamics, which requires some phenomenological choice of the jump operators⁵; $|\Psi_0\rangle$ is the ground state of the system plus bath. Two conditions are imposed. First, both discrete

⁵Deriving the jump operators from the system, bath, and system-bath coupling Hamiltonians is formally described in ch. 3 of Breuer and Petruccione [4], but is in general a highly impractical procedure.

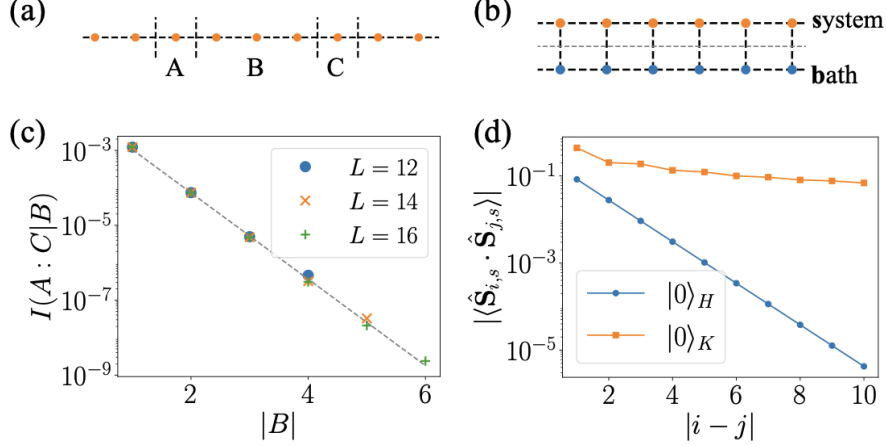


Figure 2: Fig. 2 from Ref. [3]. (a) Tripartition of a spin chain with regions A, B, and C. (b) System-bath scenario. The upper chain (system) spins have $S_s = \frac{1}{2}$ while the lower chain (bath) spins have $S_b = \frac{3}{2}$. (c) Mutual information $I(A : C | B)$ as a function of the size $|B|$. (d) Magnitude of the system spin-spin correlation $|\langle \hat{S}_{i,s} \cdot \hat{S}_{j,s} \rangle|$ versus separation $|i - j|$ in the ground states $|0\rangle_H$ of the physical Hamiltonian and $|0\rangle_K$ of the entanglement Hamiltonian.

translation and continuous spin rotation are weak symmetries, with $U^\dagger K U = K$. That is to say, the total state of the system plus bath is invariant under these symmetries. Second, it is assumed that the system spins are short-range correlated due to the coupling to the bath, with exponential decay of system spin correlations $C_{ij} = \text{Tr}(\rho S_{i,s}^z S_{j,s}^z)$ on a length scale ξ which could arise if the bath opens up a gap $\Delta \sim \xi^{-1}$ or if the system effectively thermalizes at some temperature T .

The intuition is that the system is in an ‘approximate quantum Markov state’ where the conditional mutual information shared by regions A and C separated by B (see Fig. 2(a)) is small, *i.e.* $I(A : C | B) < \varepsilon$ with ε vanishing as $\exp(-l_B/\xi)$ where l_B is the width of region B. The conditional mutual information is defined as $I(A : C | B) = I(A : BC) - I(A : B)$, where $I(A : B) = S_A + S_B - S_{AB}$ is the mutual information shared by A and B, and S_A is the von Neumann entropy of A⁶. When $I(A : C | B)$ is small, it means that B inhibits information-sharing between A and C, and when $I(A : C | B) = 0$, then $K_{ABC} = K_{AB} + K_{BC} - K_B$, which says that the entanglement Hamiltonian for the entire region ABC may be broken up into contributions from smaller regions. Zhou *et al.* conjecture that when the system is in an approximate quantum Markov state that K is exponentially local. This permits an estimate of the ‘energy’ difference $\Delta = \langle U^\dagger K U \rangle_0 - \langle K \rangle_0$, where U is the LSM twist operator and the expectation values are taken in the ground state $|0\rangle_K$ of K . A simple calculation yields this difference $\Delta \sim 4\pi^2 \xi^3 / L$ as $L \rightarrow \infty$. Since K is translationally invariant, $|0\rangle_K$ and $U|0\rangle_K$ have inequivalent crystal momenta if the system spins are all $S \in \mathbb{Z} + \frac{1}{2}$, by the LSM argument.

Zhou *et al.* study two explicit models. The first is given by

$$H = \sum_{j=1}^L \left(\mathbf{S}_j \cdot \mathbf{S}_{j+1} + \frac{1}{3} (\mathbf{S}_j \cdot \mathbf{S}_{j+1})^2 + \gamma \mathbf{S}_{j,s} \cdot \mathbf{S}_{j,b} \right) , \quad (5)$$

⁶For example, if A and B are disconnected, then $S_{AB} = S_A + S_B$ and $I(A : B) = 0$.

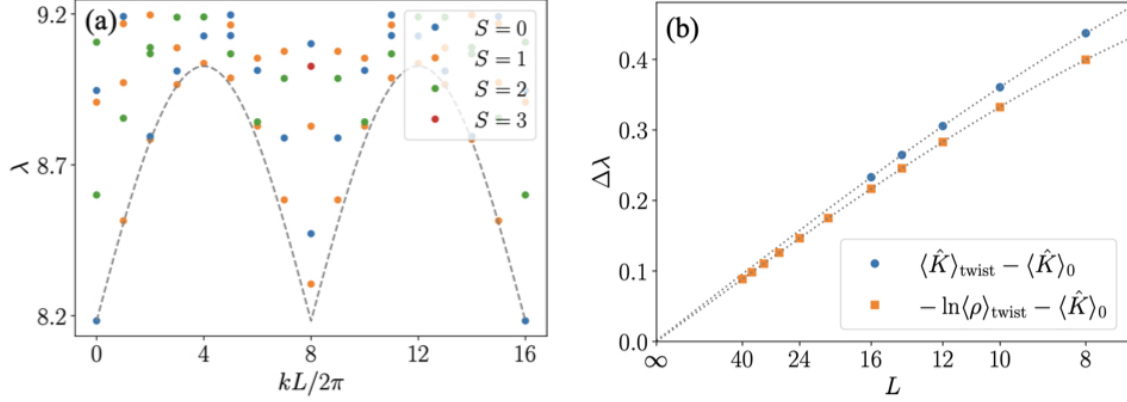


Figure 3: Fig. 3 from Ref. [3]. (a) Total spin and momentum resolved entanglement spectrum. The dashed line is given by $\lambda = v|\sin k| + \lambda_0$, with v and λ_0 fitted from the lowest eigenvalues at the lowest two momenta and $L = 16$. (b) Comparison of $\langle U^\dagger K U \rangle_0 - \langle K \rangle_0$ (blue) and $-\ln \langle U^\dagger \rho U \rangle_0 - \langle K \rangle_0$ (orange) versus L . See text for more details.

where $S_s = \frac{1}{2}$ and $S_b = \frac{3}{2}$, and $\mathbf{S}_j \equiv \mathbf{S}_{j,s} + \mathbf{S}_{j,b}$. This corresponds to the spin-ladder depicted in Fig. 2(b). When $\gamma > 0$, each rung of the ladder is preferentially in a total spin $S = 1$ state, and in this subspace remaining terms in H yield the $S = 1$ AKLT Hamiltonian [9], which exhibits a Haldane gap [10] and a spin correlation length of $\xi_{\text{AKLT}} = 1/\ln 3 \approx 0.91$. Given the exact many-body ground state in the large- γ limit, one can numerically compute the entanglement Hamiltonian K using singular value decomposition. Fig. 2(c) shows the mutual information $I(\mathbf{A} : \mathbf{C} | \mathbf{B})$, which exhibits a clear exponential decay consistent with the approximate quantum Markov state assumption. The decay length for the chosen value of γ ($= 1$?) is $\xi \approx 0.38$, which is comparable though smaller (as expected) to the AKLT result. In Fig. 3(a), the spin and momentum resolved eigenvalues λ of the entanglement Hamiltonian K are shown ($L = 16$). In Fig. 3(b) the difference $\langle U^\dagger K U \rangle_0 - \langle K \rangle_0$ is plotted versus L . It is well-fit to the curve $c_0 + c_1/L + c_3/L^3$ with $(c_0, c_1, c_3) = (0.0014, 3.8, -19)$ ⁷. The tiny values of c_0 suggest that the entanglement spectral gap vanishes in the thermodynamic limit. In addition to the Hamiltonian of Eqn. 4, another model is studied: a $S = \frac{1}{2}$ Majumdar-Ghosh chain [11] coupled to a $S = \frac{3}{2}$ bath, which yields a doubly degenerate entanglement Hamiltonian ground state separated by a robust gap from the other eigenvalues, again consistent with LSM.

It would have been illustrative to consider a $S_s = 1$ chain coupled to a bath and contrast the results with those of the two $S_s = \frac{1}{2}$ chains studied. It would seem that a form of Oshikawa's flux insertion argument should be applicable, extending the conclusions of Zhou *et al.* to dimensions $d > 1$.

I am grateful to Yi-Zhuang You for helpful discussions and for alerting me to Ref. [3].

⁷A second difference, $-\ln \langle U^\dagger \rho U \rangle_0 - \langle K \rangle_0$, which is numerically easier to compute, is also plotted.

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