Locality in Quantum and Markov Dynamics on Lattices and Networks

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We consider gapped systems governed by either quantum or Markov dynamics, with the low-lying states below the gap being approximately degenerate. For a broad class of dynamics, we prove that ground or stationary state correlation functions can be written as a piece decaying exponentially in space plus a term set by matrix elements between the low-lying states. The key to the proof is a local approximation to the negative energy, or annihilation, part of an operator in a gapped system. Applications to numerical simulation of quantum systems and to networks are discussed.

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The relation between energy and length scales is central to our understanding of physics. We intuitively associate low energies with long wavelengths. For many-body systems, at a quantum critical point, where the energy gap vanishes, we expect to see long-range correlations [1]. Conversely, experience teaches us that a gap in a quantum system implies a finite correlation length.

Such a result is well known for noninteracting systems; for example, a defect in a perfect crystal may give rise to localized modes lying within a band gap. The basic result shown in [2] is that for a large class of short-range many-body Hamiltonians this result still holds: if there is a gap between the ground and first excited states, then the connected correlation function of two operators decays exponentially in space with the correlation length ξ bounded by a characteristic velocity divided by the gap, ΔE. We note that this contrasts with the possibility of having an infinite entanglement length in a gapped system, as is studied in the field of quantum computation [3].

In this Letter, we extend this result to a more general class of systems. We consider the case of a quantum system with some number of almost degenerate low energy states, all within energy ΔE_{low} of the ground state energy, with the rest of the spectrum having an energy at least ΔE above the ground state. Then, we prove that the correlation functions include an exponentially decaying piece with correlation length ξ, plus a piece which involves matrix elements between the states below the low-lying states. The results in this Letter apply to finite range lattice Hamiltonians, with some technical conditions required to bound the group velocity on the lattice, as discussed more below. This set of systems includes short-range lattice spin systems, lattice fermion systems, and lattice hard-core boson systems. This result provides a general proof of Kohn's idea of "nearsightedness" [4] for this class of systems and thus may have important applications in $\mathcal{O}(N)$ methods for simulating quantum systems.

Proofs of some of the results used in this Letter can be found in [2]. After giving the basic results, we discuss a wide variety of applications: to systems with a band structure, to classical Markov processes, and to systems on general networks.

Consider a given connected correlation function, $\langle AB\rangle$, where A, B are operators and $\langle \cdots \rangle$ denotes the ground state expectation value. Using a spectral representation, we have $\langle AB\rangle = \sum_{E_i\leq \Delta E_{\mathrm{low}}} A_{0i}B_{i0} + \sum_{E_i\geq \Delta E} A_{0i}B_{i0}$, where i represents different intermediate states and 0 is the ground state. Define $(A_{\mathrm{low}})_{ij} = A_{ij}$ if both E_i and E_j are less than or equal to ΔE_{low}, while $(A_{\mathrm{low}})_{ij} = 0$ otherwise.

In this Letter we determine which correlation functions may be long range, given the structure of low energy states. The basic result is that for a pair of operators A, B separated by distance l, for vanishing ΔE_{low},

$$\langle AB\rangle = \langle \tfrac{1}{2}\{A_{\mathrm{low}}, B_{\mathrm{low}}\}\rangle + \mathcal{O}(\exp[-l/\xi]). \tag{1}$$

A quantum Ising system with a transverse field is a good example system to apply this result: $\mathcal{H} = J\sum_{d(i,j)\leq 1} S_i^z S_j^z + B\sum_i S_i^y$, where S_i^a are the spin operators on site i for $a = x, y, z$ and where $d(i, j)$ is some metric on the lattice. In the paramagnetic phase (B/J sufficiently large), the system has a unique ground state with a gap to the rest of the spectrum and so Eq. (1) implies that all connected correlation functions decay exponentially. In the ferromagnetic phase (B/J sufficiently small), the system has two almost degenerate low energy states and again has a gap to the rest of the spectrum. Operators such as S_i^z have long-range correlations in the ferromagnetic phase, due to matrix elements of these operators between the two low-lying states. Correlation functions of operators which do not couple the low-lying states, such as energy-energy correlation functions, are exponentially decaying.

States above the gap.—Define

$$A^{\pm} = \frac{1}{2\pi}\int_{-\infty}^{\infty} dt A(t)\frac{1}{\pm it + \epsilon}, \tag{2}$$

where $A(t) = \exp(i\mathcal{H}t)A\exp(-i\mathcal{H}t)$. Then, $(A^+)_{ij} = A_{ij}\Theta(E_i - E_j)$, where Θ is a step function: $\Theta(x) = 1$ for $x > 0$ and $\Theta(x) = 0$ for $x < 0$, while $\Theta(0) = 1/2$. Thus, A^- includes only the negative energy matrix elements of A. We may define a similar $O^{\pm}$ for any operator O.

Define $A_{\rm high} = A - A_{\rm low}$. Then,

$$\langle AB\rangle = \langle A_{\rm low}B_{\rm low}\rangle + \langle A^-_{\rm high}B\rangle = \langle A_{\rm low}B_{\rm low}\rangle + \langle [A^-_{\rm high}, B]\rangle, \tag{3}$$

since $\langle BA^-_{\rm high}\rangle = 0$. Here, we may view A^+ as a creation operator and A^- as an annihilation operator.

The basic idea of the proof in this Letter is that we will find an approximation to A^- such that we can bound both (i) the error involved in the approximation and (ii) the commutator of the approximate operator with B. By bounding both these terms, we are able to bound $\langle [A^-_{\rm high}, B]\rangle$; the reader will see later that these two considerations correspond to bounding terms in Eq. (8) below. The approximation is defined by

$$\tilde{A}(t) \equiv A(t)\exp[-(t\Delta E)^2/(2q)], \tag{4}$$

$$\tilde{A}^{\pm} = \frac{1}{2\pi}\int dt\tilde{A}(t)\frac{1}{\pm it + \epsilon}, \tag{5}$$

where q will be chosen later. In general, we may define $\tilde{O}, \tilde{O}^+$ for any operator O.

Then $(\tilde{A}^+)_{ij} = A_{ij}\Theta_q(E_i - E_j)$, where

$$\Theta_q(\omega) = \int_0^\infty \frac{d\omega'}{2\pi}(\sqrt{2\pi q}/\Delta E)\exp[-q(\omega-\omega')^2/(2\Delta E^2)]. \tag{6}$$

The function Θ_q is equal to an error function; for large q it approximates the step function Θ.

Finite group velocity.—Since A and B are separated in space, they commute. Suppose operators A, B are separated in space by a distance l, meaning that l is the shortest distance between any two sites i, j, such that some operator on site i appears in A and some operator on site j appears in B. Then, one expects that the commutator of the operators $A(t)$ and B will be small for some range of times t, with $|t|$ less than or equal to l divided by a characteristic velocity of the system. This is a bound on the group velocity [5], and the finite range of the Hamiltonian will be essential in proving it (as an example to which this result does *not* apply, a system with *long-range* Coulomb forces in two dimensions has an unbounded plasmon group velocity diverging as $1/\sqrt{q}$ for small wave vector q).

Specifically, we consider any lattice Hamiltonian $\mathcal{H}$ which can be written as a sum $\mathcal{H} = \sum_i \mathcal{H}^i$, where i ranges over lattice sites and where we require that (i) the commutator $[\mathcal{H}^i, O] = 0$ for any operator O which acts only on sites j with $d(i, j) > R$, where R is the range of the Hamiltonian, and (ii) the operator norm $\|\mathcal{H}^i\| \le J$, for all i, for some constant J. Then, it was shown in [2,5] that there exists a function $g(t, l)$, which depends on J, R, and the lattice structure, such that

$$\|[A(t), B(0)]\| \le \|A\|\|B\|\sum_j g(t, l_j) \equiv \|A\|\|B\|C(t), \tag{7}$$

where the sum ranges over sites j which appear in operator B, and $l_j = d(j, i)$ is the distance from j to the closest site i in the operator A, and where we define $C(t) = \sum_j g(t, l_j)$. It was shown that there exists some constant c_1 such that $g(c_1 l, l)$ is exponentially decaying in l for large l [2]. Further g is symmetric in t so that $g(t, l) = g(-t, l)$ and $g(t, l) \le (t/t')g(t', l)$ for $t < t'$ and $t, t' > 0$. Thus, $g(t, l)$ is monotonically increasing in t for $t > 0$. Hence, for $t \le c_1 l$, $\|[A(t), B(0)]\|$ is exponentially decaying in l for large l. We define $v \equiv c_1^{-1}$ as a velocity of the system; dimensionally, $v \propto JR$, with a lattice-dependent constant of proportionality. In a later section, we discuss the applicability of this result to systems on general graphs, or *networks*.

Commutator.—To evaluate the commutator in Eq. (3), we use

$$\langle [A^-_{\rm high}, B]\rangle = \langle [\tilde{A}^-, B]\rangle + (\langle [A^-_{\rm high}, B]\rangle - \langle [\tilde{A}^-_{\rm high}, B]\rangle) - \langle [\tilde{A}^-_{\rm low}, B]\rangle. \tag{8}$$

Here, $\tilde{A}^-_{\rm high}$ is defined by starting with $A_{\rm high}$, and then multiplying by $\exp[-(t\Delta)^2/(2q)]$, following Eq. (4), and finally taking the negative energy part. Thus, $\tilde{A}^-_{\rm high} + \tilde{A}^-_{\rm low} = \tilde{A}^-$.

First we bound the first term on the right-hand side of Eq. (8). We have

$$\begin{aligned}|\langle [\tilde{A}^-, B]\rangle| &\le \frac{1}{2\pi}\left|\int_{|t|<c_1 l} dt\exp[-(t\Delta E)^2/(2q)]\langle [A(t), B]\rangle\frac{1}{-it+\epsilon}\right| + \frac{1}{2\pi}\left|\int_{|t|>c_1 l} dt\exp[-(t\Delta E)^2/(2q)]\langle [A(t), B]\rangle\frac{1}{-it+\epsilon}\right| \\ &\le \frac{1}{2\pi}\|A\|\|B\|\left[2C(c_1 l) + 2\frac{\sqrt{2\pi q}}{\Delta E c_1 l}e^{-(c_1 l\Delta E)^2/(2q)}\right].\end{aligned} \tag{9}$$

In Eq. (9), for $|t| < c_1 l$, we have used $\exp[-(t\Delta E)^2/(2q)]\langle [A(t), B\rangle] \le \|[A(t), B]\|$ and Eq. (7), while for $|t| > c_1 l$ we have used $\exp[-(t\Delta E)^2/(2q)]\langle [A(t), B\rangle] \le 2\exp[-(t\Delta E)^2/(2q)]\|A\|\|B\|$ and have performed the integrations using these bounds.

Next, we consider the second pair of terms on the right-hand of Eq. (8). From Eq. (6) it follows that, for $|\omega| \ge \Delta E$, $|\Theta_q(\omega) - \Theta(\omega)| \le \exp[-q/2]/\sqrt{2\pi q}$. Thus, if $\Psi_0\rangle$ is the ground state wave function, $|\langle\Psi_0 A^-_{\rm high} - \langle\Psi_0\tilde{A}^-_{\rm high}| \le \|A\|\exp[-q/2]/\sqrt{2\pi q}$, and also $|A^-_{\rm high}\Psi_0\rangle - \tilde{A}^-_{\rm high}\Psi_0\rangle| \le \|A\|\exp[-q/2]/\sqrt{2\pi q}$. Then,

$$|\langle [A^-_{\rm high}, B]\rangle - \langle [\tilde{A}^-_{\rm high}, B]\rangle| \le 2\|A\|\|B\|\frac{\exp[-q/2]}{\sqrt{2\pi q}}. \tag{10}$$

Physically, Eq. (10) is a kind of uncertainty relation: the time integral in Eq. (4) extends over a time of order $\sqrt{q}\Delta E^{-1}$ and thus provides an approximation to energies of order $\Delta E/\sqrt{q}$.

Almost degenerate low energy states.—Suppose $\Delta E_{\rm low}$ is very small compared to ΔE. Then, for $\omega \leq \Delta E_{\rm low}$, $\Theta_q(\omega)$ is close to 1/2: $|\Theta_q(\omega) - 1/2| \leq \sqrt{q/2\pi}(\omega/\Delta E)$. Thus, $|\langle[\tilde{A}^-_{\rm low}, B]\rangle - \frac{1}{2}\langle[A_{\rm low}, B]\rangle| \leq 2\|A_{\rm low}\|\|B_{\rm low}\| \times \sqrt{q/2\pi}(\omega/\Delta E)$. Then, from Eqs. (3) and (8)–(10) above, it follows that

$$|\langle AB\rangle - \langle A_{\rm low}B_{\rm low}\rangle - \frac{1}{2}\langle[A_{\rm low}, B_{\rm low}]\rangle| \leq 2\|A\|B\|\left(\frac{C(c_1 l)}{2\pi} + \frac{\sqrt{q}}{2\pi\Delta E c_1 l}\exp[-(c_1 l\Delta E)^2/(2q)] + \frac{\exp[-q/2]}{\sqrt{2\pi q}}\right) + 2\|A_{\rm low}\|\|B_{\rm low}\|\sqrt{q/2\pi}(\Delta E_{\rm low}/\Delta E). \tag{11}$$

Equation (11) is valid for any q. Picking $q = c_1 l\Delta E$ to get the tightest bound, we have

$$\left|\langle AB\rangle - \left\langle\frac{1}{2}\{A_{\rm low}, B_{\rm low}\}\right\rangle\right| \leq \|A\|\|B\|\left[2C(c_1 l)/(2\pi) + \frac{4}{\sqrt{2\pi q}}e^{-c_1 l\Delta E/2}\right] + 2\|A_{\rm low}\|\|B_{\rm low}\|\sqrt{c_1 l\Delta E/2\pi}(\Delta E_{\rm low}/\Delta E). \tag{12}$$

The first term in brackets in Eq. (12) is exponentially decaying in l with some correlation length ξ_C. The second term in brackets decays exponentially with correlation length $2/(c_1\Delta E)$. Thus, we define the correlation length ξ to be the minimum of ξ_C and $2/(c_1\Delta E)$. For $\Delta E_{\rm low}$ taken to be zero, we have Eq. (1).

Low energy commutator.—We can also bound the expectation value $\langle[A_{\rm low}, B_{\rm low}]\rangle$. Define $\tilde{A}^0 = \Delta E/\sqrt{2\pi q} \times \int_{-\infty}^{\infty} dt\tilde{A}(t)$. Then, we can bound the commutator: $|\langle[\tilde{A}^0, B]\rangle| \leq \Delta E/\sqrt{2\pi q}\{\int_{|t|<c_1 l} dt C(t) + |\int_{|t|>c_1 l} dt\langle[\tilde{A}(t), B]\rangle|\} \leq \|A\|\|B\|\{\sqrt{c_1 l\Delta E/2\pi}C(c_1 l) + 2e^{-c_1 l\Delta E/2}\}$. Next, consider the difference $\langle[\tilde{A}^0, B]\rangle - \langle[A_{\rm low}, B_{\rm low}]\rangle$. This equals $(\langle[\tilde{A}^0_{\rm low}, B\rangle - \langle[A_{\rm low}, B_{\rm low}]\rangle) + \langle[\tilde{A}^0_{\rm high}, B]\rangle$. Explicit computation with a spectral representation gives $|\langle[\tilde{A}^0_{\rm low}, B]\rangle - \langle[A_{\rm low}, B_{\rm low}]\rangle| \leq 2\|A_{\rm low}\|\,\|B_{\rm low}\|\,(e^{-q(\Delta E_{\rm low}/\Delta E)^2/2} - 1)$, while $|\langle[\tilde{A}^0_{\rm high}, B]\rangle| \leq 2\|A\|B\|e^{-c_1 l\Delta E/2}$. Combining these bounds with the bound on $|\langle[\tilde{A}^0, B]\rangle|$ gives

$$|\langle[A_{\rm low}, B_{\rm low}]\rangle| \leq \|A\|\|B\|[\sqrt{c_1 l\Delta E/2\pi}C(c_1 l) + 4e^{-c_1 l\Delta E/2}] + 2\|A_{\rm low}\|\|B_{\rm low}\|(e^{-q(\Delta E_{\rm low}/\Delta E)^2/2} - 1). \tag{13}$$

Thus, for $\Delta E_{\rm low} = 0$, we find that $|\langle[A_{\rm low}, B_{\rm low}]\rangle|$ is exponentially decaying in l.

Operators at different times.—We finally extend the result Eq. (12) to correlation functions $\langle A(-i\tau)B(0)\rangle$, with τ real and $\tau > 0$. Define

$$\tilde{A}^{\pm}(\pm i\tau) = \frac{1}{2\pi}\int dt\tilde{A}(t)\frac{1}{\pm it + \tau} \tag{14}$$

by $-it + \tau$. In this case, we find that Eq. (9) still holds as a bound for $|\langle[\tilde{A}^-(-i\tau), B]\rangle|$. One may also show that, for $\tau \leq q/\Delta E$, $|\langle[\tilde{A}^-_{\rm high}(-i\tau), B]\rangle - \exp[+\tau^2\Delta E^2/(2q)] \times \langle[A^-_{\rm high}(-i\tau), B]\rangle| \leq 2\|\|\|B\|e^{-q/2}$.

With the given $q = c_1 l\Delta E$ the above bounds show that for $\tau \leq c_1 l$,

$$|\langle A(-i\tau)B(0)\rangle - \langle A_{\rm low}(-i\tau)B_{\rm low}(0)\rangle| \leq e^{-\tau^2\Delta E/(2c_1 l)}\left[\frac{1}{2\pi}2\|A\|\|B\|C(c_1 l) + \left(2 + \frac{2}{\sqrt{2\pi q}}\right)\|A\|\|B\|e^{-c_1\Delta E l/2} + |\langle[\tilde{A}^-_{\rm low}(-i\tau), B]\rangle|\right]. \tag{15}$$

To bound the last term in the above equation, we use $\|A_{\rm low}(t) - A_{\rm low}(0)\| \leq t\Delta E_{\rm low}\|A_{\rm low}\|$. Define $z = (2\pi)^{-1} \times \int dt\exp[-(t\Delta E)^2/(2q)]/(-it + \tau)$. Then, $|\langle[\tilde{A}^-_{\rm low}(-i\tau), B]\rangle - z\langle[A_{\rm low}, B_{\rm low}]\rangle| \leq \pi^{-1}\int dt t\Delta E_{\rm low}\|A_{\rm low}\|\|B_{\rm low}\| \times \exp[-(t\Delta E)^2/(2q)]/(-it + \tau) \leq \sqrt{2q/\pi}\|A_{\rm low}\|\|B_{\rm low}\| \times (\Delta E_{\rm low}/\Delta E)$. Thus, for $\Delta E_{\rm low} = 0$, $|\langle[\tilde{A}^-_{\rm low}(-i\tau), B]\rangle|$ is exponentially decaying in l, following Eq. (13).

Band structure.—These techniques can also be applied to problems with a band structure. All of the results above can be generalized to fermionic operators A, B by interchanging commutators and anticommutators throughout. Consider a free fermionic theory, with spectrum with two bands separated by a band gap $2\Delta E$. Then, we can shift the zero of energy so that the spectrum has some set of states with energy at most $-\Delta E$ and another with energy at least ΔE. Then, if $A = \psi_i^\dagger$ is the fermionic creation operator at some point i, we can define an operator $\tilde{A}^-$ which approximately projects $\psi_i^\dagger$ onto the lower band. At the same time, $\tilde{A}^-$ will be exponentially localized around point i, so that $\|\{\tilde{A}^-, O\}\| = \mathcal{O}(\exp[-(c_1 l\Delta E)^2/(2q)]) + \mathcal{O}(C(c_1 l))$, if the fermionic operator O acts only on a site j with $d(x, j) = l$. This approximation may be useful for computing the density matrix in these systems[6]: if the chemical potential is such that all states are filled up to zero energy, then $\rho(i, j) \equiv \langle\psi_i^\dagger\psi_j\rangle = \langle\{A^-, \psi_j\}\rangle \approx \langle\{\tilde{A}^-, \psi_j\}\rangle$.

Markov processes.—The above locality results can also be carried over to systems which obey continuous time dynamics, following [2], where we have a transition matrix T_{ij} and a probability p_i of being in state i, so that $\partial_t p_i = \sum_j T_{ij} p_j$. By conservation of total probability, we have $\sum_i T_{ij} = 0$, guaranteeing that T has at least one zero eigenvalue. Let this stationary state with zero eigenvalue have right eigenvector p_i^0 and left eigenvector I_i; here, $I_i = 1$ for all i.

Suppose all eigenvalues of T are real (this includes all systems for which the stationary state obeys detailed balance). All eigenvalues of T are nonpositive. Then, assume that there are some number of eigenvalues λ_i of T with $0 \geq \lambda_i \geq -\Delta_{\rm low}$, while all other eigenvalues λ_i have $\lambda_i \leq -\Delta$, with $\Delta > \Delta_{\rm low}$. For each quantity to be measured, $A, B, \ldots,$ define $\langle A \rangle = \sum_i A_i p_i^0$. We can introduce for each quantity a diagonal matrix given by $\hat{A}_{ii} = A_i$, and $\hat{A}_{ij} = 0$ for $i \neq j$. Then, $\langle A(t) B(0) \rangle = I^\dagger \exp[-Tt] \times \hat{A} \exp[Tt] \hat{B} p^0 \equiv I^\dagger \hat{A}(t) B p^0$. We have left off the indices on the vector I, p and on the matrices $\hat{A}, \hat{B}, \exp[\pm Tt]$; the product is evaluated following the usual rules of matrix multiplication. We can continue these definitions of $A(t)$ to *imaginary time* and define $\tilde{A}(it) = \hat{A}(it) \times \exp[-(t\Delta)^2/(2q)]$ while $\tilde{A}^+ = \frac{1}{2\pi} \int dt \tilde{A}(it)(\mp it + \epsilon)^{-1}$.

Assume that T can be written as a sum of matrices T^i, with finite interaction range R and bound $\|T^i\| \leq J$ for all i. With these preliminaries, all of the above manipulations can be carried out for Markov processes. In particular, $\langle AB \rangle = \langle (1/2)\{A_{\rm low}, B_{\rm low}\} \rangle + \mathcal{O}(\exp[-l/\xi])$.

Networks.—Recently, systems on general graphs or *networks* have been studied much [7]. Example systems include the random graph and the small-world network [8]. Locality is an important question in these systems, for community detection, for example [9,10]. In a small world, the presence of long-range jumps can completely destroy locality above some length scale so that all critical behavior is mean field [11].

Following [2], the bound Eq. (7) holds for any graph for which all sites have a bounded number of neighbors (counting a neighbor as any other site within distance R) and for which $|T^i| \leq J$ for all sites i. This includes a large class of interesting networks, such as the small-world network. However, another large class of interesting networks, the scale-free networks, has an unbounded coordination number. In many of these cases, $\mathcal{H}$ (or T) can be written as a sum of operators lying on bonds which have bounded operator norm. Then, we can add to the graph a set of additional sites which lie on these bonds between sites on the original network, calling one of new these sites (i, j) if it lies on the bond between i and j. Then, we can let $\mathcal{H} = \sum_{(i,j)} \mathcal{H}^{(i,j)}$, with $\|\mathcal{H}^{(i,j)}\| \leq J$.

However, we still must deal with the unbounded number of neighbors. The range of one of these bond Hamiltonians is such that (i, j) is within range R of (i, k) for all j, k which neighbor i, so that we cannot bound the number of neighbors within range of a given bond (i, j). However, if the given scale-free networks is *loopless*, inspection of the proof in [2] shows that Eq. (7) still holds. Thus, we claim that for networks with either bounded coordination number and bounded $\mathcal{H}^i$ or loopless networks with bounded $\mathcal{H}^{ij}$, the result Eq. (1) is valid.

As an example, consider the contact process for epidemic spreading [12] on a small-world network. Away from the critical point, in the endemic phase, the Markov process governing the dynamics of this process has a gapped transition matrix. Then, a correlation function of the number of infected individuals on a site i with the number on a site j decays exponentially as $\exp[-d(i, j)/\xi]$, where $d(i, j)$ is the shortest path distance from i to j.

Discussion.—The result we have shown is expected on physical grounds. In a gapped system, the correlation function can be written as in Eq. (1): an exponentially decaying piece, plus a piece determined by matrix elements between the low-lying states. In the quantum Ising system of the introduction, the local operator S_i^z has nonvanishing matrix elements between two low-lying states. In a fractional quantum Hall system with a topological degeneracy and a gap to the rest of the spectrum [13], the matrix elements between the low-lying states are small for all local operators, so all correlation functions decay exponentially. Finally, in the spin-1/2 antiferromagnet on the Kagomé lattice, which appears to have a divergent but subextensive number of low energy spin singlets lying below a finite gap [14], only singlet operators may have long range correlations.

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