Spin Gases: Quantum Entanglement Driven by Classical Kinematics

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A spin gas is a natural extension of a classical gas. It consists of a large number of particles whose (random) motion is described classically, but, in addition, have internal (quantum mechanical) degrees of freedom that interact during collisions. For specific types of quantum interactions we determine the entanglement that occurs naturally in such systems. We analyze how the evolution of the quantum state is determined by the underlying classical kinematics of the gas. For the Boltzmann gas, we calculate the rate at which entanglement is produced and characterize the entanglement properties of the equilibrium state.

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We study the entanglement properties of spin gases. We define a spin gas as a system of interacting spins (or qubits) where the coupling strengths between the spins are stochastic functions of time. A system that could serve as a textbook example of a spin gas is the semiquantal Boltzmann gas, where each particle carries an internal (two-level) quantum degree of freedom. During a collision of two particles, the internal degrees of freedom interact and can become entangled. The statistics of the collisions, described by kinetic gas theory, leads to randomly fluctuating coupling strengths between the spins. It is an intriguing question, how the evolution of the quantum state of the system is determined by the underlying classical thermodynamics of the gas. What kind of entanglement is created in the gas and at which rate? How is the equilibrium state of the gas characterized in terms of its entanglement? In this Letter we will give an answer to these and to other questions, which make the study of spin gases interesting both from the perspective of thermodynamics and of quantum information.

Spin gases differ from spin lattices in that the coupling strengths have no translational symmetry and evolve in time. From a formal point of view, spin gases are more closely related to spin glasses, which have random, albeit static, couplings between the spins. Although there has been much recent work investigating, e.g., the role of entanglement in quantum critical phenomena [see, e.g., [1–4]], there is little work studying disordered quantum systems from a similar perspective [see, however, [5]].

We give a simple, and yet realistic, collision model for the particles carrying the spins, and study the quantum mechanical states that emerge from the dynamics of such a spin gas, which we also refer to as a *semiquantal gas*. In full generality, this problem seems intractable for various reasons: the description of a many-body quantum state usually requires exponentially large resources; strong interactions do not allow for a perturbative treatment; random interactions prevent the appearance of symmetries and the corresponding reduction of the effective number of degrees of freedom; finally, the restriction to low-energy eigenspaces, suitable for the study of ground-state or low-temperature properties, cannot be applied here to the study of dynamics. State-of-the-art numerical methods are limited to systems of moderate size (up to a few hundred particles) with an entanglement that is bound or scales at most with the surface of the block [6]. However, in disordered quantum systems with random interactions, such as the spin gas studied here, entanglement will typically increase with the volume of the block. Nevertheless, for Ising (or, more generally, commuting two-body) interactions we can calculate the full dynamics of the many-body state exactly, and efficiently compute its bipartite and multipartite entanglement properties.

Formal preliminaries.—We consider a situation where N particles move along some classical trajectories $\boldsymbol{r}_k(t)$, while their quantum degrees of freedom interact according to a distance- and time-dependent Hamiltonian

$$H(t) = \sum_{k<l} g[\boldsymbol{r}_k(t), \boldsymbol{r}_l(t)] H^{(kl)}, \tag{1}$$

where the function $g[\boldsymbol{r}_k(t), \boldsymbol{r}_l(t)]$ is determined by the particular two-body interaction. We restrict ourselves to specific types of interactions, namely, those where all $H^{(kl)}$ commute. Consequently, we find that after a time t the initial state $|\Psi_0\rangle$ evolves to

$$|\Psi_t\rangle = U_t|\Psi_0\rangle = \prod_{k>l} U^{(kl)}[\varphi_{kl}(t)]|\Psi_0\rangle, \tag{2}$$

with $U^{(kl)}[\varphi_{kl}(t)] = e^{-i\varphi_{kl}(t)H^{(kl)}}$ and $\varphi_{kl}(t) = \int_0^t g[\boldsymbol{r}_k(t'), \boldsymbol{r}_l(t')]dt'$. At time t, the quantum state is fully determined by the $N(N-1)/2$ phases $\varphi_{kl}(t)$, which in turn are determined by the interaction history of the N particles. Each phase can be interpreted as a matrix element $\Gamma_{kl} = \varphi_{kl}$ of an adjacency matrix $\Gamma(t)$ defining a weighted graph. This description allows one to use graph-theoretical terms, such as average path length, giant components, clustering coefficient, or connectivity in the study of entanglement in spin gases (see discussion on localizable entanglement below). In this work we focus on the Boltzmann gas in a regime

where the so-called random or Erdős-Rényi graphs [7] appear. Other models of spin gases [e.g., [8]] can give rise to graphs, such as small worlds graphs [9], with further interesting properties.

We now focus our attention on the case of an Ising-type interaction with $H^{(kl)} = |11\rangle_{kl}\langle 11|$. We assume that all particles are initially prepared in the internal state $|+\rangle = 1/\sqrt{2}(|0\rangle + |1\rangle)$, and interact only upon a collision. These restrictions are made for simplicity, but similar methods can be applied to general commuting $H^{(kl)}$, and arbitrary $g[\boldsymbol{r}_k(t), \boldsymbol{r}_l(t)]$ and initial states (without additional overhead).

The evolution of the initial state $|\Psi_0\rangle = |+\rangle^{\otimes N}$ can be described in the standard basis $\{|0\rangle, |1\rangle\}^{\otimes N}$,

$$U_t|+\rangle^{\otimes N} = 2^{-N/2}\sum_{\mathbf{s}} U_t|\mathbf{s}\rangle = 2^{-N/2}\sum_{\mathbf{s}} e^{i/2\mathbf{s}\cdot\Gamma(t)\cdot\mathbf{s}}|\mathbf{s}\rangle, \quad (3)$$

where the sum is carried out over all N-digit binary vectors $\mathbf{s}$, i.e., over all 2^N different combinations of zeros and ones. We emphasize that all the time dependence is contained in the adjacency matrix $\Gamma(t)$ of the graph. The parametrization of the quantum state in terms of a weighted graph that summarizes the ''collisional history'' of the gas is both intuitive and useful for our calculations.

Many properties of this global pure state can be understood in terms of the reduced density matrices of its subsystems. Since the unitary operations in (2) commute with each other, the evolution of a set A of N_A particles can be separated into two contributions. The first entangles particles within A and is determined by the block Γ_{AA} of the adjacency matrix. The second contribution couples the subsystem A to the rest B of the system through the off-diagonal block Γ_{AB}. The effect of the latter can be obtained by tracing out the set of particles B from the state $|\Psi_t\rangle$:

$$\begin{aligned}\tilde{\rho}_A &= \frac{1}{2^N}\,\mathrm{tr}_B \sum_{\mathbf{s},\mathbf{s}'}^{2^N-1} e^{i1/2(\mathbf{s}.\Gamma.\mathbf{s}-\mathbf{s}'\cdot\Gamma\cdot\mathbf{s}')}|\mathbf{s}\rangle\langle\mathbf{s}'| \\ &= \frac{1}{2^{N_A}}\sum_{\mathbf{s}_A,\mathbf{s}'_A}\left(\frac{1}{2^{N_B}}\sum_{\mathbf{s}_B} e^{i(\mathbf{s}_A-\mathbf{s}'_A)\cdot\Gamma_{AB}\cdot\mathbf{s}_B}\right)|\mathbf{s}_A\rangle\langle\mathbf{s}'_A|. \quad (4)\end{aligned}$$

The second equality is obtained by writing $|s\rangle = |s_A\rangle|s_B\rangle$, and the tilde in $\tilde{\rho}_A$ indicates that interactions within subsystem A are not taken into account (Γ_{AA} is set to zero). Clearly, the values of the block Γ_{BB} do not affect the properties of either ρ_A or $\tilde{\rho}_A$. In the standard basis, each off-diagonal element—or ''coherence''—of the initial state is decreased by a factor, $\tilde{\rho}_{s_A s'_A}(t) = C_{s_A s'_A}\tilde{\rho}_{s_A s'_A}(0)$, while diagonal elements remain untouched. The multiplying factor can be conveniently written as

$$C_{s_A s'_A} = e^{i/2\sum_k (\mathbf{s}_A-\mathbf{s}'_A)\cdot\Gamma_{\mathbf{k}}}\prod_{k=1}^{N_B}\cos\left[\frac{1}{2}(\mathbf{s}_A-\mathbf{s}'_A)\cdot\Gamma_{\mathbf{k}}\right], \quad (5)$$

where we have defined the N_A-dimensional vector $(\Gamma_{\mathbf{k}})_j = \Gamma_{kj}$ for each particle $k \in B$ [10]. In this form, we see that the total effect of the interactions with particles in B on a particular coherence of ρ_A can be obtained by multiplying the effects of each individual particle in B. More succinctly, if $\rho_A^{(k)}$ is the state of the subsystem due to the sole effect of particle $k \in B$, then the state ρ_A is obtained (up to normalization) by the *Hadamard product* of all $\{\rho_A^{(k)}\}_{k=1}^{N_B}$ written in the standard basis, that is, by their componentwise multiplication. This observation was also made in [11] within the context of valence bond solids.

The decomposition into Hadamard products allows one to read off the matrix elements of ρ_A from the adjacency matrix, but most importantly it signifies that one can efficiently compute [8] reduced density operators ρ_A of small subsystems A, even when the size N of the total system is essentially arbitrarily large. The computational effort scales only linearly with N_B in contrast to the general case where the computational resources to calculate ρ_A scale exponentially with N_B (because the partial trace has to be performed over all 2^{N_B} basis states in B).

The time dependence of the quantum state of the system in terms of $\Gamma(t)$ (3), together with the efficient method (5) to compute the state of (small) subsystems are crucial properties that allow us to study spin gases. For a complete characterization of the dynamics, one still needs to find, for each particular gas model, the behavior of the stochastic function $\Gamma(t)$. This task amounts to assigning a probability $p_{\Gamma(t)}$ to every collisional history $\Gamma(t)$. However, in order to calculate the evolution of average properties as we do here, it is enough to have the probability distribution $p_t(\Gamma)$ of the Γ's at time t. Depending on the parameter regime, semiquantal gases can follow various collision patterns and accordingly exhibit drastically different dynamics of their quantum properties.

Characterization of entanglement.—Whereas entanglement of bipartite systems is rather well understood, entanglement properties of multipartite systems are in general difficult to determine. However, for pure global states, we can already get a broad picture of the entanglement in a multipartite system by considering all possible 2^{N-1} splits of the set of particles in two groups (A and B). The entanglement properties with respect to such bipartitions A-B are completely determined by the eigenvalues of the reduced density operator $\rho_A = \mathrm{tr}_B|\Psi_t\rangle\langle\Psi_t|$, and one can use the entropy of entanglement $S_A = -\mathrm{tr}(\rho_A \log_2 \rho_A)$ to quantify them. However, the calculation of reduced density matrices is, in general, very difficult if not impossible (exponential scaling in both N_A and N_B). Even to ascertain whether a given system is entangled or not [rank $(\rho_A) > 1$ or $= 1$] may be impossible. For states $|\Psi_t\rangle$ that occur in the spin gases under consideration, many of these restrictions do not apply. First, we can use (5) to determine in an efficient way the density matrix ρ_A of small subsystems A and hence calculate the entropy of entanglement with respect to all such bipartitions. We can also compute quantities such as the multipartite Meyer-Wallach pure-state entanglement measure [12], which only depends on single-body density matrices, or the ''correlation

strengths'' [13] for finite blocks, or classical correlation functions like those used in generalized n-party Bell inequalities [14]. Second, we have a simple criterion for the presence of entanglement: the state $|\Psi_t\rangle$ is entangled with respect to the partition A-B *iff* the two groups are connected (i.e., an interaction between some particle in A and some particle in B has taken place) [8].

A different aspect of (global) multipartite entanglement is the question whether entanglement can be created (localized) between two arbitrary subsets of particles A_1-A_2 by performing *local* operations on the other particles. For states arising in the spin gas, we find that this is the situation *iff* there exists a path between A_1 and A_2 in the corresponding graph, in which case their localizable entanglement [4] is nonzero.

In the following, we illustrate the above methods by studying the dynamics of entanglement in the specific case of a semiquantal Boltzmann gas.

Boltzmann gas.—We consider a dilute ideal gas of N particles in thermal equilibrium with a mean free path comparable to the size of the enclosing volume. The statistical state of the gas is fully specified by the density n, the volume V, and the temperature T. We assume Stosszahlansatz (or molecular chaos) and hence take a homogeneous and uncorrelated spatial distribution of the particles (density), and an uncorrelated velocity distribution. The latter is given by the Maxwell-Boltzmann distribution and is characterized by the single parameter $\sigma = \sqrt{k_B T/m}$, where m is the mass of the particles and k_B the Boltzmann constant. We assume a hard-sphere model for collisions between particles of diameter d and that at every collision particles acquire a phase inversely proportional to their relative velocity, $\varphi_{kl} = \gamma/v_{kl}$. We study entanglement that arises if at a given time $t = 0$ all spins are polarized along the x axis, i.e., $|+\rangle$.

We first note that in such gas the quantum state is specified at every time by a *random graph* [7] with weighted edges. Random graphs are known to exhibit a phase transition as the average degree z of a vertex increases. This is reflected, e.g., in the creation of *entangled clusters*—or, following the graph-theory nomenclature, entangled components—that is, subsets of particles that are connected in the graph, such that entanglement can be localized between any of the constituent particles. Initially, one finds that small $[O(\log N)]$ entangled clusters emerge, but after a time t such that $z = rt = 1$ (where r is the collision rate) a system-sized $[O(N)]$ *giant component* [7] appears, equivalent to percolation in infinite dimensions. Hence, any pair of particles will be (with high probability) localizable entangled after a finite time, even for $N \to \infty$.

One could compute entanglement properties by direct simulation of the Boltzmann gas as done elsewhere for a lattice gas [8]. Here, however, we will focus on regimes where analytical results can be obtained, namely, for large collisional phases and arbitrary times, or for arbitrary phases in the limits of short and infinite times.

In a regime of large collisional phases $\phi \sim \gamma\sigma^{-1} \gg 1$ (i.e., large interaction constant or low temperatures) we can assign to each collision event a random phase in $[0, 2\pi]$. This already allows us to find the expected entropy for short times $rt < 1$, where $r = \pi d^2 n \langle v_r \rangle$ is the collision rate and $\langle v_r \rangle = \sqrt{16KT/(m\pi)}$ is the mean relative velocity. For these short times, a particle will typically collide at most once (with probability rt), and the resulting expected entropy can be obtained by direct integration: $\frac{1}{2\pi} \int S(\phi) d\phi = 2 - \log_2 e$. Hence, we find $\langle S_1 \rangle = rt(2 - \log_2 e) + \mathcal{O}[(rt)^2]$. The entropy of entanglement between a block A of size N_A and the rest of the system B can be obtained by counting the average number of collisions that occur between particles of A and B:

$$\langle S_A \rangle \approx \frac{N_A N_B}{N-1} rt(2 - \log_2 e) \quad \text{for } rt < 1. \tag{6}$$

For arbitrary times, we can obtain a lower bound to the von Neumann entropy using the following sequence of inequalities: $\langle S_A \rangle \geq -\langle \log_2(\mathrm{tr}\, \rho_A^2) \rangle \geq -\log_2(\langle \mathrm{tr}\, \tilde{\rho}_A^2 \rangle) = -\log_2(\sum_{s_A, s_A'} \langle |C_{s_A, s_A'}|^2 \rangle / 2^{2N_A})$. From (5) we notice that the coherence $C_{s_A, s_A'}$ only depends on the difference $\mathbf{z}_A = \mathbf{s}_A - \mathbf{s}_A'$. And, in particular, the average $\langle |C_{s_A, s_A'}|^2 \rangle$ depends only on the number Z_A of nonzero entries of $\mathbf{z}_A$. Each particle k in B will contribute with a factor $1/2$ to the product in (5) if it has collided with at least one particle of the subset of A where $\mathbf{z}_A$ has nonzero entries, whereas a factor one appears otherwise. Since the probability that no such collision occurs is $p_{z_A} = \exp(-rtZ_A/N)$, each term in the product will contribute on average with a factor $1/2(1 - p_{z_A}) + p_{z_A} = [1 + \exp(-rtZ_A/N)]/2$. Taking into account combinatoric factors we arrive at

$$\langle S_A(t) \rangle \geq -\log_2 \left[\frac{1}{2^N} \sum_{Z_A=0}^{N_A} \binom{N_A}{Z_A} (1 + e^{-rtZ_A/(N-1)})^{N_B} \right].$$

Numerical results for $N_A \leq 8$ and arbitrary system sizes $(N_A + N_B)$ show that this lower bound is also a good estimate and describes well the behavior of the entropic entanglement. This lower bound can be supplemented by the upper bound $\langle S_A \rangle \leq N_A \langle S_1 \rangle$. The latter follows from the subadditivity property of the von Neumann entropy.

In the short- or long-time limits we can simplify the above expression for the entanglement between two arbitrary parts of the Boltzmann gas. For short times $rtN_A/(N-1) < 1$

$$\langle S_A(t) \rangle \geq -\log_2 \left(1 - \frac{N_A N_B}{4(N-1)} rt \right) \approx \frac{N_A N_B}{4 \ln 2 (N-1)} rt,$$

which is consistent with the exact result (6) for short times.

In the long-time limit all particles will have collided with all other particles many times and accumulated phases $\varphi_{kl} \gg 1$, independently of the collisional phase per collision. We refer to such a state as the *equilibrium* state. For sufficiently large times, $rt \gg N$, every term with $Z_A > 0$ in

the sum (7) approaches one (disregarding the binomial factor) while the $Z_A = 0$ term is equal to two,

$$\langle S_A \rangle \geq -\log_2\left(\frac{1}{2^{N_A}} + \frac{1}{2^{N_B}} - \frac{1}{2^N} + \frac{N_A N_B}{2^N} e^{-rt/(N-1)}\right).$$

The equilibrium state ($rt \to \infty$) has thus the interesting feature that $|\Psi_\infty\rangle$ is maximally entangled with respect to *all* possible bipartitions, i.e., $S_A \approx N_A$, provided that the total number of particles N in the gas is sufficiently large. This is a nontrivial statement especially in the case where both partitions are similarly large. For whatever bipartition one takes, we find that the expected entropy of entanglement is at most a single bit away from its maximal value: $N_A \geq \langle S_A \rangle > N_A - 1$. This result is in agreement with the findings of Page [15] and subsequent work studying average or typical entanglement properties of the whole set of multipartite pure states. Another remarkable property of the equilibrium state is that the localizable entanglement between *any* pair of particles approaches its maximum value of one e-bit as N increases [8]. Although the dynamics of the entanglement strongly depends on the particular type and regime of the semiquantal gas, the equilibrium state will, in general, be of the form we just described.

To conclude our analysis, we consider the regime of small collisional phases in the short-time limit. In this regime, we have to take into account the relative velocity of the colliding partners. A calculation involving standard kinetic-theory arguments shows that at short times ($rt \ll 1$) the expected value for the squared modulus of the coherence is given by the expression

$$\langle |C_{01}|^2 \rangle_t \approx 1 - tn\pi d^2 \int dv\, p_r(v) v (1 - |C_v|^2) = 1 - \alpha t,$$

where $p_r(v)$ is the relative velocity distribution and $|C_v| = \cos[\phi(v)/2]$ is the modulus of the velocity dependent coherence. For small phases $\gamma\sigma^{-1} < 1$ the proportionality factor α can be approximated by

$$\alpha = \frac{4\pi^2 d^2 n}{(4\pi\sigma^2)^{3/2}} \int dv\, v^3 e^{-v^2/4\sigma^2} \sin^2\left(\frac{\gamma}{2v}\right) \approx \frac{1}{4} n\sqrt{\pi} d^2 \frac{\gamma^2}{\sigma}.$$

Following the previous reasoning we find

$$\langle S_A(t) \rangle \geq -\frac{N_A N_B}{N-1} \log_2\left(1 - \frac{\alpha}{2} t\right) \approx \frac{\alpha}{2\ln 2} \frac{N_A N_B}{N-1} t. \quad (7)$$

Thus, by writing $\alpha \approx \frac{1}{4}\sqrt{m\pi} d^2 \gamma^2 \frac{n}{\sqrt{k_B T}}$ we obtain the rate of entanglement generation in terms of the thermodynamical variables. Whereas in the regime of large collisional phases entanglement grows with the rate of collisions ($\propto \sqrt{T}$), for small collisional phases we find that entanglement generation is governed by the slow collision events (larger phases) leading to the opposite behavior ($\alpha \propto \sqrt{T^{-1}}$).

Summary.—In this Letter we studied the stochastic generation of entanglement in a spin gas, in which the classical kinematics of the particles drives the quantum state of the many-body system. The spin gas provides a novel scenario to study relationships between classical thermodynamical variables and properties of the quantum state of the system, such as quantum correlations, rate of entanglement generation, equilibrium values, and clustering effects. We have shown how to formalize such systems under quite general conditions and examined in detail the case of the semiquantal Boltzmann gas. We have fully characterized the bipartite aspects of the entangled N-body equilibrium state, which is reached at long enough times for most gas models, showing that maximum entanglement is asymptotically attained for all possible bipartitions. The same formalism can also be used [8] to conduct efficient simulations of other semiquantal gases, such as lattice gases, with a large number of particles ($N \sim 10^5$) that exhibit nontrivial features like non-Markovian dynamics or highly correlated collision patterns.

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