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Propagation of Molecular Chaos by Quantum Systems and the Dynamics of the Curie-Weiss Model

Alexander Gottlieb

Abstract

The propagation of molecular chaos, a tool of classical kinetic theory, is generalized to apply to quantum systems of distinguishable particles. We prove that the Curie-Weiss model of ferromagnetism propagates molecular chaos and derive the effective dynamics of a single-spin state in the mean-field limit. Our treatment differs from the traditional approach to mean-field spin models in that it concerns the dynamics of single-particle states instead of the dynamics of infinite-particle states.

1 Introduction

The infinite-particle dynamics of spin models with finite-range interactions — such as the Ising model — can be defined without difficulty in the norm limit of the local (finite-particle) dynamics [21][Section 7.6]. For mean-field spin models such as the Curie-Weiss model, the infinite-particle dynamics can only be defined in certain *representations* of the infinite-particle algebra, as the limit in the strong operator topology of the local dynamics [6, 1]. The purpose of this note is to introduce a new approach to the quantum mean-field dynamics via the propagation of quantum molecular chaos. The concept of quantum molecular chaos enables us to comprehend the infinite-particle limit of the Curie-Weiss dynamics without constructing an infinite-particle dynamics.

For classical mean-field systems, the theory of the propagation of molecular chaos enables one to study the effective dynamics of finite groups of particles without defining dynamics of infinite particle states. We can achieve the same end in the quantum context by utilizing the analog for quantum systems of theory of the propagation of molecular chaos. This device is exploited in [19], where a quantum version of propagation of molecular chaos is used to derive the Vlaosov equation from the dynamics of quantum particles in the continuum. Their approach was inspired by [3], wherein the Vlasov equation was derived from the propagation of molecular chaos by mean-field systems of *classical* particles.

The concept of molecular chaos dates back to Boltzmann [2]. In order to derive the fundamental equation of the kinetic theory of gases, Boltzamnn assumed that the molecules of a nonequilibrium gas were in a state of "molecular disorder." Nowadays, the term "molecular chaos" connotes a system of classical particles that may be regarded as having stochastically independent and identically distributed random positions and momenta. The state of any molecularly chaotic system is characterized by the probability law of a single particle of the system, and so the temporal evolution of any system that is at all times in a state of molecular chaos reduces to that of the probability law of a *single* particle. Both Boltzmann's equation for dilute gases and Vlasov's equation for dilute plasmas may be interpreted as equations that describe the dynamics of the position-velocity distribution $f(\mathbf{x},\mathbf{v})d\mathbf{x}d\mathbf{v}$ of a single particle in a molecularly chaotic gas or plasma. Because gases and plasmas remain in a molecularly chaotic state once they have entered one, i.e., because they "propagate molecular chaos," the kinetic equations of Boltzmann and Vlasov can be thought of as evolution equations for a single-particle distribution $f(\mathbf{x},\mathbf{v})d\mathbf{x}d\mathbf{v}$.

The concept of *propagation* of molecular chaos is due to Kac [11, 12], who called it "propagation of the Boltzmann property" and used it to derive the homogenous Boltzmann equation from the infinite particle asymptotics of certain Markovian gas models. This idea was further developed in work by [9, 16, 26, 23]. McKean [14, 15] proved the propagation of chaos by systems of interacting diffusions. See [3, 24, 20, 5, 8] for more recent work on and some generalizations of McKean's propagation of chaos. For two good surveys of propagation of chaos and its applications, see [25, 17].

This paper is organized as follows. Quantum molecular chaos is defined in Section 2, and related to classical molecular chaos. Examples of quantum molecular chaos are provided; it is shown that sequences of canonical states are often molecularly chaotic. In Section 3 we define the propagation of quantum molecular chaos. We then prove that the Curie-Weiss model propagates molecular chaos and solve the mean-field dynamical equation for the single-particle state.

2 Quantum Molecular Chaos

The definition of molecular chaos current in the probability literature is equivalent to the following [25, 7]:

Definition 1 *Let S be a separable metric space. For each $n \in \mathbb{N}$, let ρ_n be a symmetric probability measure on S^n, the n-fold Cartesian power of S. ("Symmetric" means that the measures of rectangles are invariant under permutations of the coordinate axes.) Let ρ be a probability measure on S.*

*The sequence $\{\rho_n\}$ is ρ-**chaotic** if the k-dimensional marginal distributions $\rho_n^{(k)}$ converge (weakly) to $\rho^{\otimes k}$ as $n \longrightarrow \infty$, for each fixed $k \in \mathbb{N}$.*

The quantum analog of a probability measure is a state on a C*-algebra with identity. A *state* on a C*-algebra with identity $\mathcal{A}$ is a positive linear functional on $\mathcal{A}$ that equals 1 at the identity element. The space of states on $\mathcal{A}$ endowed with the weak* topology will be denoted $\mathcal{S}(\mathcal{A})$. Molecular chaos is an attribute of certain sequences of symmetric probability measures; we now define *quantum* molecular chaos to be an attribute of certain sequences of symmetric states.

Definition 2 (Quantum Molecular Chaos) *Let $\mathcal{A}$ be a C*-algebra with identity, and denote the n-th (spatial) tensor power of $\mathcal{A}$ by $\otimes^n \mathcal{A}$. Let ρ be a state on $\mathcal{A}$. For each $n \in \mathbb{N}$, let ρ_n be a symmetric state on $\otimes^n \mathcal{A}$, that is, a state on $\otimes^n \mathcal{A}$ that satisfies*

$$\rho_n(A_1 \otimes \cdots \otimes A_n) = \rho_n(A_{\pi(1)} \otimes \mathcal{A}_{\pi(2)} \otimes \cdots \otimes A_{\pi(n)})$$

for all permutations π of $\{1, 2, \ldots, n\}$. For each $k \leq n$, let $\rho_n^{(k)} \in \mathcal{S}(\otimes^k \mathcal{A})$ be defined by

$$\rho_n^{(k)}(B) = \rho_n(B \otimes \mathbf{1} \otimes \mathbf{1} \otimes \cdots \otimes \mathbf{1}),$$

for all $B \in \otimes^k \mathcal{A}$, and let $\rho^{\otimes k}$ be defined by the condition that, for all $A_1, A_2, \ldots, A_k \in \mathcal{A}$,

$$\rho^{\otimes k}(A_1 \otimes A_2 \otimes \cdots \otimes A_k) = \rho(A_1)\rho(A_2) \cdots \rho(A_k).$$

*The sequence $\{\rho_n\}$ is ρ-**chaotic** if, for each $k \in \mathbb{N}$, the states $\rho_n^{(k)}$ converge weakly* to $\rho^{\otimes k}$ in $\mathcal{S}(\otimes^k \mathcal{A})$ as $n \longrightarrow \infty$.*

*The sequence $\{\rho_n\}$ is **molecularly chaotic** if it is ρ-chaotic for some state ρ on $\mathcal{A}$.*

Suppose $\mathcal{A}$ is the algebra generated by the observables for a single particle of a certain species. The algebra generated by all single-particle observables in a system of n *distinguishable* particles of the same species is $\otimes^n\mathcal{A}$, and states on $\otimes^n\mathcal{A}$ correspond to statistical ensembles of those n-particle systems. Quantum molecular chaos of a sequence of n-particle states expresses a condition of quasi-independence of the particles when the number of particles is very large.

Quantum molecular chaos is related to classical molecular chaos as follows:

Theorem 1 *Let $\mathcal{A}$ be a C^* algebra with identity $\mathbf{1}$ and for each $n \in \mathbb{N}$ let ρ_n be a symmetric state on $\otimes^n\mathcal{A}$. The following are equivalent:*

(i) The sequence $\{\rho_n\}$ is ρ-chaotic in the sense of Definition 2.

(ii) For each pair of positive elements Q_0 and Q_1 satisfying $Q_0 + Q_1 = \mathbf{1}$, the sequence of probability measures $\{P_n\}$ on $\{0,1\}^n$ defined by

$$P_n(j_1, j_2, \ldots, j_n) = \rho_n(Q_{j_1} \otimes Q_{j_2} \otimes \cdots \otimes Q_{j_n}),$$

is P-chaotic in the classical sense of Definition 1, where P is the probability measure on $\{0,1\}$ defined by

$$P(j) = \rho(Q_j).$$

Proof:

It is clear from Definition 2 that (i) $\Longrightarrow$ (ii). The rest of this proof is devoted to showing that (i) $\Longrightarrow$ (ii).

We first establish the following claim: Let $\mathcal{P}(\mathcal{S}(\mathcal{A}))$ denote the space of regular Borel probability measures on the state space of $\mathcal{A}$, endowed with the weak* topology as the dual of $C(\mathcal{S}(\mathcal{A}))$. Let σ be any state on $\mathcal{A}$. The measure δ_σ, a point mass at σ, is is the only measure $\mu \in \mathcal{P}(\mathcal{S}(\mathcal{A}))$ such that

$$\mu\{\tau \in \mathcal{S}(\mathcal{A}) : |\tau(Q) - \sigma(Q)| \geq \epsilon\} = 0 \tag{1}$$

for every $\epsilon > 0$ and $Q \in \mathcal{A}$ with $\mathbf{0} \leq Q \leq \mathbf{1}$. To prove this claim, first note that (1) holds for *every* element of $\mathcal{A}$ if it holds for those elements Q with $\mathbf{0} \leq Q \leq \mathbf{1}$, since every element of $\mathcal{A}$ is a linear combination of such positive elements. Since (1) holds for every $Q \in \mathcal{A}$, the Borel measure μ is supported on arbitrarily small basic open neigborhoods of $\sigma \in \mathcal{S}(\mathcal{A})$, whence it follows that $\mu(\{\sigma\}) = 1$, since μ is a regular measure.

Next we define a couple of homeomorphisms: Let $\otimes^\infty\mathcal{A}$ denote the inductive limit of the spatial tensor products $\otimes^n\mathcal{A}$. A state $\sigma \in \otimes^\infty\mathcal{A}$ is called *symmetric* if

$$\begin{aligned} & \sigma(A_1 \otimes A_2 \otimes \cdots \otimes A_n \otimes \mathbf{1} \otimes \mathbf{1} \otimes \cdots) \\ = \quad & \sigma(A_{\pi(1)} \otimes A_{\pi(2)} \otimes \cdots \otimes A_{\pi(k)} \otimes A_{k+1} \otimes \cdots \otimes A_n \otimes \mathbf{1} \otimes \mathbf{1} \otimes \cdots) \end{aligned}$$

for all elements $A_1, A_2, \dots, A_n$ of $\mathcal{A}$, and all permutations π of $\{1, 2, \dots, k\}$, $k \leq n$. Denote the space of symmetric states on $\otimes^\infty\mathcal{A}$ by $\mathcal{S}_{sym}(\otimes^\infty\mathcal{A})$. Størmer's theorem [22][Theorem 2.8] states that there exists an affine homeomorphism Φ from the space $\mathcal{P}(\mathcal{S}(\mathcal{A}))$ of regular probability measures on $\mathcal{S}(\mathcal{A})$ to $\mathcal{S}_{sym}(\otimes^\infty\mathcal{A})$, such that $\Phi(\delta_\mu) = \mu^{\otimes\infty}$. The classical precursor of Størmer's theorem, de Finetti's theorem [10], states that there exists an affine homeomorphism $\Xi : \mathcal{P}(\mathcal{P}(\{0,1\})) \longrightarrow \mathcal{P}_{sym}(\{0,1\}^\infty)$ such that $\Xi(\delta_p) = p^{\otimes\infty}$.

Now assume that condition (ii) holds.

Let τ be an arbitrary but fixed state on $\mathcal{A}$, and for each n, extend $\rho_n \in \otimes^n\mathcal{A}$ to the state

$$\tilde{\rho}_n = \rho_n \otimes \tau \otimes \tau \otimes \tau \otimes \tau \otimes \tau \otimes \cdots$$

in $\mathcal{S}(\otimes^\infty\mathcal{A})$ Since $\mathcal{S}(\otimes^\infty\mathcal{A})$ is weak* compact, every subsequence of $\{\tilde{\rho}_n\}$ has cluster points; condition (ii) will used to prove that $\rho^{\otimes\infty}$ is the *only* cluster point of $\{\tilde{\rho}_n\}$. It will follow that $\{\tilde{\rho}_n\}$ converges to $\rho^{\otimes\infty}$, which implies that $\{\rho_n\}$ is ρ-chaotic.

Let $\mu \in \mathcal{S}(\otimes^\infty\mathcal{A})$ be any cluster point of $\{\tilde{\rho}_n\}$, the limit of the subsequence $\{\tilde{\rho}_{n_k}\}$. Because of the increasing symmetry of the $\tilde{\rho}_{n_k}$, the state μ is symmetric: $\mu \in \mathcal{S}_{sym}(\otimes^\infty\mathcal{A})$. Suppose that $\mu \neq \rho^{\otimes\infty}$ (this assumption will lead to a contradiction). Then $\Phi^{-1}(\mu) \neq \delta_\rho$ and we have shown that there must exist $\mathbf{0} < Q < \mathbf{1}$ and $\epsilon > 0$ such that

$$\Phi^{-1}(\mu)\{\sigma : |\sigma(Q) - \rho(Q)| \geq \epsilon\} > 0. \tag{2}$$

Set $Q_0 = Q$ and $Q_1 = \mathbf{1} - Q$. Define $P : \mathcal{S}(\mathcal{A}) \longrightarrow \mathcal{P}(\{0,1\})$, mapping σ to P_σ, by

$$P_\sigma(j) = \sigma(Q_j)\ ; \quad j \in \{0,1\}.$$

Define $P^\infty : \mathcal{S}(\otimes^\infty\mathcal{A}) \longrightarrow \mathcal{P}(\{0,1\}^\infty)$, mapping σ to P^∞_σ, by

$$P^\infty_\sigma\{(x_1, x_2, \dots) : x_1 = j_1, \dots, x_n = j_n\} = \sigma(Q_{j_1} \otimes \cdots \otimes Q_{j_n} \otimes \mathbf{1} \otimes \cdots).$$

Condition (ii) implies that $P^\infty(\tilde{\rho}_{n_k}) \longrightarrow (P_\rho)^{\otimes\infty}$. Since P^∞ is continuous and $\tilde{\rho}_{n_k} \longrightarrow \mu$, it follows that

$$P^\infty(\mu) = (P_\rho)^{\otimes\infty}. \tag{3}$$

The composite map $\Xi^{-1} \circ P^\infty \circ \Phi$ is affine and continuous, and it maps δ_σ to δ_{P_σ} for every $\sigma \in \mathcal{S}(\mathcal{A})$. The map $\widetilde{P} : \mathcal{P}(\mathcal{S}(\mathcal{A})) \longrightarrow \mathcal{P}(\mathcal{P}(\{0,1\}))$ induced by $P : \mathcal{S}(\mathcal{A}) \longrightarrow \mathcal{P}(\{0,1\})$ is also affine and continuous, and also maps δ_σ to δ_{P_σ} for every $\sigma \in \mathcal{S}(\mathcal{A})$, so $\widetilde{P}$ must equal $\Xi^{-1} \circ P^\infty \circ \Phi$ by the Krein-Milman theorem. That is, the following diagram commutes:

$$\begin{array}{ccc}
\mathcal{P}(\mathcal{S}(\mathcal{A})) & \xrightarrow{\Phi} & \mathcal{S}_{sym}(\otimes^\infty \mathcal{A}) \\
{\scriptstyle \widetilde{P}}\downarrow & & \downarrow{\scriptstyle P^\infty} \\
\mathcal{P}(\mathcal{P}(\{0,1\})) & \xrightarrow{\Xi} & \mathcal{P}_{sym}(\{0,1\}^\infty)
\end{array}$$

By equation (3) and the commutativity of the preceding diagram,

$$\widetilde{P}(\Phi^{-1}(\mu)) = \Xi^{-1}(P^\infty(\mu)) = \delta_{P_\rho}. \tag{4}$$

But equation (2) implies that

$$\widetilde{P}(\Phi^{-1}(\mu))\{p \in \mathcal{P}(\{0,1\}) : |p(0) - P_\rho(0)| \geq \epsilon\} > 0,$$

and this contradicts (4).
■

Corollary 1 *Let $\mathcal{A}$ be a C^* algebra with identity, and for each $n \in \mathbb{N}$ let ρ_n be a symmetric state on $\otimes^n \mathcal{A}$. If $\rho_n^{(2)}$ converges to $\rho \otimes \rho$ then $\{\rho_n\}$ is ρ-chaotic.*

Proof:

Let Q_0 and Q_1 be any positive elements of $\mathcal{A}$ such that $Q_0 + Q_1 = \mathbf{1}$, and let P_n and P be as in the statement of Theorem 1. The measures P_n are symmetric, and $P_n^{(2)}$ converges to $P \otimes P$ since $\rho_n^{(2)}$ converges to $\rho \otimes \rho$. This suffices to imply that $\{P_n\}$ is P-chaotic [25]. The ρ-chaos of $\{\rho_n\}$ now follows from Theorem 1.
■

The following theorem shows that sequences of canonical states for mean-field systems are often molecularly chaotic:

Theorem 2 *Let V be an operator on $\mathbb{C}^d$ such that $V(x \otimes y) = V(y \otimes x)$ for all $x, y \in \mathbb{C}^d$. Let $V^n_{1,2}$ denote the operator on $\otimes^n \mathbb{C}^d$ defined by*

$$V^n_{1,2}(x_1 \otimes x_2 \otimes \cdots \otimes x_n) = V(x_1 \otimes x_2) \otimes x_3 \otimes \cdots \otimes x_n,$$

and for each $i < j \leq n$, define V^n_{ij} as acting similarly on the i^{th} and j^{th} factors of each simple tensor. Define the states $\rho_n \in \mathcal{S}(\otimes^n \mathbb{C}^d)$ by

$$\rho_n(A) = \tfrac{1}{Z}\mathrm{Tr}\left(e^{-H_n} A\right) \;; \qquad H_n = \tfrac{1}{n}\sum_{i<j} V^n_{ij} \;; \qquad Z = \mathrm{Tr}\left(e^{-H_n}\right).$$

The sequence $\{\rho_n\}$ is ρ-chaotic if the density operator for ρ is the unique minimizer of the free energy

$$F[D] = \frac{1}{2}\mathrm{Tr}((D \otimes D)V) + \mathrm{Tr}(D \log D).$$

If V is positive definite then F has a unique minimizer.

Proof Sketch: This theorem is the quantum version of Theorems 2 and 4 of [18]. The properties of classical entropy that Messer and Spohn used to prove those theorems are equally true for the von Neumann entropy $-\mathrm{Tr}(D \log D)$ of density operators, at least when D operates on $\mathbb{C}^d$. The necessary properties of von Neumann entropy are proved in [13].
□

3 The Curie-Weiss Model Propagates Chaos

A sequence of n-particle dynamics "propagates chaos" if molecularly chaotic sequences of initial distributions remain molecularly chaotic for all time under the n-particle dynamical evolutions.

In the classical context, the n-particle dynamics are Markovian. Accordingly, in [7], we defined propagation of chaos in terms of Markov transition functions:

Definition 3 *For each $n \in \mathbb{N}$, let $K_n : S^n \times \sigma(S^n) \times [0, \infty) \longrightarrow [0, 1]$ be a Markov transition function which commutes with permutations in the sense that*

$$K_n(\mathbf{x}, E, t) = K_n(\pi \cdot \mathbf{x}, \pi \cdot E, t)$$

for all permutations π of the n coordinates of $\mathbf{x}$ and the points of $E \subset S^n$, and for all $t \geq 0$. (Here, $\sigma(S^n)$ denotes the Borel σ-field of S^n.)

The sequence $\{K_n\}_{n=1}^{\infty}$ **propagates chaos** *if, for all* $t \geq 0$*, the molecular chaos of a sequence* $\{\rho_n\}$ *entails the molecular chaos of the sequence* $\left\{\int_{S^n} K_n(\mathbf{x}, \cdot, t)\rho_n(d\mathbf{x})\right\}$.

The quantum analog of a Markov transition function is a completely positive unital map. A linear map $\phi : \mathcal{A}_1 \longrightarrow \mathcal{A}_2$ of C* algebras is *completely positive* if, for each $n \in \mathbb{N}$, the map from $\mathcal{A}_1 \otimes \mathcal{B}(\mathbb{C}^n)$ to $\mathcal{A}_2 \otimes \mathcal{B}(\mathbb{C}^n)$ that sends $A \otimes B$ to $\phi(A) \otimes B$ is positive [4]. Propagation of chaos is an attribute of certain sequences of Markov transition functions; we now define *quantum* propagation of chaos to be an attribute of certain sequences of completely positive unital maps.

Definition 4 (Propagation of Quantum Molecular Chaos) *For each* $n \in \mathbb{N}$*, let* ϕ_n *be a completely positive map from* $\otimes^n \mathcal{A}$ *to itself that fixes the unit* $\mathbf{1} \otimes \cdots \otimes \mathbf{1} \in \otimes^n \mathcal{A}$ *and which commutes with permutations, i.e., such that*

$$\phi_n(A_{\pi(1)} \otimes A_{\pi(2)} \otimes \cdots \otimes A_{\pi(n)}) = \pi \cdot \phi_n(A_1 \otimes A_2 \otimes \cdots \otimes A_n) \tag{5}$$

for all permutations π *of* $\{1, 2, \ldots, n\}$*, where* $\pi\cdot$ *denotes the operator on* $\otimes^n \mathcal{A}$ *defined by*

$$\pi \cdot (B_1 \otimes B_2 \otimes \cdots \otimes B_n) = B_{\pi(1)} \otimes B_{\pi(2)} \otimes \cdots \otimes B_{\pi(n)}$$

for all $B_1, B_2, \ldots, B_n \in \mathcal{A}$.

The sequence $\{\phi_n\}$ **propagates chaos** *if the molecular chaos of a sequence of states* $\{\rho_n\}$ *entails the molecular chaos of the sequence* $\{\rho_n \circ \phi_n\}$.

Consider the case where $\mathcal{A}$ is the algebra generated by the observables for a single particle of a certain species, so that $\otimes^n \mathcal{A}$ is the algebra generated by all single-particle observables in a system of n *distinguishable* particles of that species. For each $n \in \mathbb{N}$, let the dynamics of the n-particle system be given by a Hamiltonian operator $H_n \in \otimes^n \mathcal{A}$. In the Heisenberg version of quantum dynamics, if A is the operator that corresponds to measurement of a certain observable quantity at $t = 0$, the operator corresponding to the measurement of the same quantity at time $t > 0$ equals $e^{iH_n t/\hbar} A e^{-iH_n t/\hbar}$. The maps $\phi_{n,t} : \otimes^n \mathcal{A} \to \otimes^n \mathcal{A}$ defined by

$$\phi_{n,t}(A) = e^{iH_n t/\hbar} A e^{-iH_n t/\hbar} \tag{6}$$

are completely positive, and if they satisfy condition (5) one may ask whether the sequence $\{\phi_{n,t}\}$ propagates chaos.

We conjecture that chaos always propagates when the n-particle Hamiltonians H_n are as follows: Let $\mathcal{A} = \mathcal{B}(\mathbb{C}^d)$, the algebra of all bounded operators on $\mathbb{C}^d$. The algebra $\otimes^n \mathcal{A}$ is isomorphic to $\mathcal{B}(\otimes^n \mathbb{C}^d)$, and states $\tau \in \mathcal{S}(\otimes^n \mathcal{A})$ correspond to density operators D_τ on $\mathcal{B}(\otimes^n \mathbb{C}^d)$ via the equation $\tau(A) = \mathrm{Tr}(D_\tau A)$. Suppose that V is a Hermitian operator on $\mathbb{C}^d \otimes \mathbb{C}^d$ that is symmetric in the sense that $V(x \otimes y) = V(y \otimes x)$ for all $x, y \in \mathbb{C}^d$. Let $V_{1,2}^n$ denote the operator on $\otimes^n \mathbb{C}^d$ defined by

$$V_{1,2}^n(x_1 \otimes x_2 \otimes \cdots \otimes x_n) = V(x_1 \otimes x_2) \otimes x_3 \otimes \cdots \otimes x_n,$$

and for each $i < j \leq n$, define V_{ij}^n similarly (as acting on the i^{th} and j^{th} factors of each simple tensor). Define the n-particle Hamiltonian H_n as the sum of the pair potentials V_{ij}^n, with a $1/n$ scaling of the coupling constant:

$$H_n = \frac{1}{n} \sum_{i<j} V_{ij}^n. \tag{7}$$

Conjecture 1 *The sequence $\{\phi_{n,t}\}$ defined in equation (6) propagates chaos:*

If $\{\rho_n\}$ is ρ-chaotic then $\{\rho_n \circ \phi_{n,t}\}$ is ρ_t-chaotic, where the density operator for ρ_t is the solution at time t of

$$\begin{aligned} \frac{\partial}{\partial t} D &= -\frac{i}{\hbar}[V, D \otimes D]^{(1)} \\ D(0) &= D_\rho. \end{aligned} \tag{8}$$

Here $[V, D \otimes D]^{(1)}$ denotes a contraction of $[V, D \otimes D]$: if $\{y_i\}$ is any orthonormal basis of $\mathbb{C}^d$ and $x \in \mathbb{C}^d$,

$$[V, D \otimes D]^{(1)}(x) = \sum_i < [V, D \otimes D](x \otimes y_i), (x \otimes y_i) > .$$

This conjecture will now be verified for the Curie-Weiss model of ferromagnetism. In this model, the ferromagnetic material is modelled by a crystal in which the spin angular momentum of each atom is coupled to the average spin and to an external magnetic field. In case the applied magnetic field is directed along the z-axis, we may make the approximation that only the z-components of the spins are coupled to each other and the external field. As in [6, 1], we consider the case of spin-$\frac{1}{2}$ atoms, so that the space of pure spin states of a single particle is $\mathbb{C}^2$, and the observables corresponding to the measurement of the x, y and z components of spin are the Pauli spin operators

$$\sigma^x = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \sigma^y = \frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad \sigma^z = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

The space of pure states of an n-spin system is $\otimes^n \mathbb{C}^2$. For each $i \leq n$, if A is an operator on $\mathbb{C}$, let A_i denote the operator on $\otimes^n \mathbb{C}^2$ defined by

$$A_i(v_1 \otimes v_2 \otimes \cdots \otimes v_n) = v_1 \otimes \cdots \otimes A(v_i) \otimes \cdots \otimes v_n.$$

If A is Hermitian, A_i corresponds to the measurement of the spin observable A at the i^{th} lattice site. The Hamiltonian for the n-site Curie-Weiss model is

$$\mathcal{H}_n = -J \sum_{i=1}^{n} \left(\sigma_i^z \frac{\sum_j \sigma_j^z}{n} \right) - H \sum_{i=1}^{n} \sigma_i^z = \frac{1}{n} \sum_{i,j=1}^{n} \left(-J\sigma_i^z \sigma_j^z - H\sigma_i^z \right),$$

where J is a positive coupling constant and H is another constant proportional to the strength of the external magnetic field.

Since $\otimes^n \mathcal{B}(\mathbb{C}^2)$ is isomorphic to $\mathcal{B}(\otimes^n \mathbb{C}^2)$, states $\rho_n \in \mathcal{S}(\otimes^n \mathcal{B}(\mathbb{C}^2))$ correspond to density operators D_{ρ_n} in $\otimes^n \mathbb{C}^2$. ¿From definition (6) and the fact that $\mathrm{Tr}(AB) = \mathrm{Tr}(BA)$,

$$\begin{aligned} \rho_n \circ \phi_{n,t}(A) &= \mathrm{Tr}(D_{\rho_n} e^{i\mathcal{H}_n t/\hbar} A e^{-i\mathcal{H}_n t/\hbar}) \\ &= \mathrm{Tr}(e^{-i\mathcal{H}_n t/\hbar} D_{\rho_n} e^{i\mathcal{H}_n t/\hbar} A). \end{aligned}$$

Therefore, $\rho_n \circ \phi_{n,t}$ has the density operator

$$D_{\rho_n \circ \phi_{n,t}} = e^{-i\mathcal{H}_n t/\hbar} D_{\rho_n} e^{i\mathcal{H}_n t/\hbar}. \tag{9}$$

For any state ρ on $\mathcal{B}(\mathbb{C}^2)$, let D_ρ denote the corresponding density operator, and let $\left[D_{\rho(t)}\right]$ denote a 2×2 matrix that represents D_ρ.

Theorem 3 *The sequence of Hamiltonians $\{\mathcal{H}_n\}$ propagates chaos. If $\{\rho_n\}$ is a ρ-chaotic sequence of states with $[D_\rho] = \begin{pmatrix} a & c \\ \bar{c} & d \end{pmatrix}$, then for each $t \geq 0$, $\{\rho_n \circ \phi_{n,t}\}$ is $\rho(t)$-chaotic, where*

$$\left[D_{\rho(t)}\right] = \begin{pmatrix} a & ce^{it(H+\hbar J(a-d))} \\ \bar{c}e^{-it(H+\hbar J(a-d))} & d \end{pmatrix}.$$

Proof of Theorem 3:

If $\mathbf{x} \in \{0,1\}^n$ for some $n \in \mathbb{N}$, let $\mathcal{N}(\mathbf{x})$ denote the number of 1s in $\mathbf{x}$:

$$\mathcal{N}(\mathbf{x}) = \sum_{i=1}^{n} x_i$$

if $\mathbf{x} = (x_1, x_2, \ldots, x_n)$. If $g : \{0,1\}^n \longrightarrow \mathbb{C}$ is a symmetric function, then $g(\mathbf{x})$ depends on $\mathbf{x}$ only through $\mathcal{N}(\mathbf{x})$, so that $g(\mathbf{x}) = g(\mathbf{y})$ if $\mathcal{N}(\mathbf{x}) = \mathcal{N}(\mathbf{y})$.

Lemma 1 *For each $n \in \mathbb{N}$, let $f_n : \{0,1\}^n \longrightarrow \mathbb{C}$ be a symmetric function. Suppose that*

(a) there exists $B < \infty$ such that $\sum_{\mathbf{s}\in\{0,1\}^n} |f_n(\mathbf{s})| \leq B$ for all n, and

(b) there exists $c \in \mathbb{C}$ and $f : \{0,1\} \longrightarrow \mathbb{C}$ such that, for $k = 0, 1, 2, \ldots$,

$$\sum_{z_1, z_2, \ldots, z_{n-k}} f_n(x_1, \ldots, x_k, z_1, \ldots, z_{n-k}) \longrightarrow c f(x_1) f(x_2) \cdots f(x_k)$$

as $n \longrightarrow \infty$.

Then

(i) For all $G \in C_{\mathbb{C}}([0,1])$,

$$\lim_{n\to\infty} \sum_{\mathbf{x}\in\{0,1\}^n} f_n(\mathbf{x}) G\left(\frac{\mathcal{N}(\mathbf{x})}{n}\right) = c\ G(f(1))$$

(ii) If $c \neq 0$ then $0 \leq f(0), f(1) \leq 1$ and $f(0) + f(1) = 1$.

Proof of Lemma: Let

$$F_n(j) = \sum_{\mathcal{N}(\mathbf{x})=j} f_n(\mathbf{x}). \tag{10}$$

Condition (b) implies that

$$\lim_{n\to\infty} \sum_{z_1, z_2, \ldots, z_{n-k}} f_n(1, 1, \ldots, 1, z_1, \ldots, z_{n-k}) = c\,(f(1))^k$$

for all $k \in \mathbb{N}$. Grouping the summands for which exactly j coordinates of $(1, 1, \ldots, 1, z_1, \ldots, z_{n-k})$ equal 1, we find that

$$\lim_{n\to\infty} \sum_{j=k}^{n} F_n(j) \frac{\begin{pmatrix} n-k \\ j-k \end{pmatrix}}{\begin{pmatrix} n \\ j \end{pmatrix}} = c\,(f(1))^k. \tag{11}$$

Now

$$\sum_{j=k}^{n} F_n(j) \frac{\begin{pmatrix} n-k \\ j-k \end{pmatrix}}{\begin{pmatrix} n \\ j \end{pmatrix}} = \sum_{j=k}^{n} F_n(j) \frac{j(j-1)\cdots(j-k+1)}{n(n-1)\cdots(n-k+1)},$$

while

$$\begin{aligned}
&\left| \sum_{j=k}^{n} F_n(j) \frac{j(j-1)\cdots(j-k+1)}{n(n-1)\cdots(n-k+1)} - \sum_{j=0}^{n} F_n(j) \left(\frac{j}{n}\right)^k \right| \\
\leq \;& \sum_{j=0}^{n} |F_n(j)| \left(\left(\frac{k}{n}\right)^n + \max_{j \geq k} \left\{ \left| \frac{j(j-1)\cdots(j-k+1)}{n(n-1)\cdots(n-k+1)} - \left(\frac{j}{n}\right)^k \right| \right\} \right) \\
\leq \;& B \left[\left(\frac{k}{n}\right)^n + \max_{j \geq k} \left\{ \left(\frac{j}{n}\right)^k - \left(\frac{j-k+1}{n}\right)^k \right\} \right] \\
\leq \;& B \left[\left(\frac{k}{n}\right)^n + \frac{1}{n^k} \max_{j \geq k} \left\{ \begin{pmatrix} k \\ 1 \end{pmatrix} j^{k-1}(k-1) + \begin{pmatrix} k \\ 2 \end{pmatrix} j^{k-2}(k-1)^2 + \cdots + (k-1)^k \right\} \right] \\
\leq \;& B \left[\left(\frac{k}{n}\right)^n + \frac{1}{n} \left\{ \begin{pmatrix} k \\ 1 \end{pmatrix} k + \begin{pmatrix} k \\ 2 \end{pmatrix} k^2 + \cdots + k^k \right\} \right] \\
\leq \;& B \left[\left(\frac{k}{n}\right)^n + \frac{1}{n}(1+k)^k \right],
\end{aligned}$$

and therefore

$$\lim_{n\to\infty} \sum_{j=k}^{n} F_n(j) \frac{\begin{pmatrix} n-k \\ j-k \end{pmatrix}}{\begin{pmatrix} n \\ j \end{pmatrix}} = \lim_{n\to\infty} \sum_{j=0}^{n} F_n(j) \left(\frac{j}{n}\right)^k. \tag{12}$$

Condition (a) implies that $\sum_j |F_n(j)| \leq B$ for all n. This bound, equations (11) and (12), and the fact that any continuous function on $[0,1]$ can be approximated uniformly by polynomials, imply that

$$\lim_{n\to\infty} \sum_{j=0}^{n} F_n(j) G\left(\frac{j}{n}\right) = c\; G\left(f(1)\right)$$

for all $G \in C_{\mathbb{C}}([0,1])$. This establishes (i), in view of the definition (10) of F_n.

If $c \neq 0$, conclusion (i) implies that $f(1) \in [0,1]$. Condition (b) for $k=0$ and $k=1$ states that

$$\begin{aligned}
\lim_{n\to\infty} \sum_{z_1,z_2,\dots,z_n} f_n(z_1,z_2,\dots,z_n) &= c \\
\lim_{n\to\infty} \sum_{z_1,z_2,\dots,z_{n-1}} f_n(1,z_1,\dots,z_{n-1}) &= cf(1) \\
\lim_{n\to\infty} \sum_{z_1,z_2,\dots,z_{n-1}} f_n(0,z_1,\dots,z_{n-1}) &= cf(0),
\end{aligned}$$

so it follows that $f(0)+f(1)=1$ if $c \neq 0$. This establishes (ii), concluding the proof of the lemma.
■

Let $e_1=(1,0)$ and $e_2=(0,1)$. For each $n \in \mathbb{N}$, let

$$\mathcal{E}_n = \left\{ e_{j_1} \otimes e_{j_2} \otimes \cdots \otimes e_{j_n} \in \otimes^n \mathbb{C}^2 \middle| \; j_1, j_2, \dots, j_n \in \{1,2\} \right\}.$$

Denote by $[A]^{k_1,\dots,k_n}_{j_1,\dots,j_n}$ the matrix elements for an operator A on $\otimes^n\mathbb{C}^2$ relative to the basis $\mathcal{E}_n$, that is, for $j_1,k_1,\dots,j_n,k_n \in \{1,2\}$, let

$$[A]^{k_1,\dots,k_n}_{j_1,\dots,j_n} = \langle A(e_{j_1}\otimes e_{j_2}\otimes\cdots\otimes e_{j_n}), e_{k_1}\otimes e_{k_2}\otimes\cdots\otimes e_{k_n}\rangle .$$

The sequence $\{\rho_n\}$ is ρ-chaotic. This implies that, for each $k \in \mathbb{N}$,

$$\sum_{z_1,z_2,\dots,z_{n-k}\in\{1,2\}} [D_{\rho_n}]^{y_1,\dots,y_k,z_1,\dots,z_{n-k}}_{x_1,\dots,x_k,z_1,\dots,z_{n-k}} \longrightarrow [D_\rho]^{y_1}_{x_1}[D_\rho]^{y_2}_{x_2}\cdots[D_\rho]^{y_k}_{x_k},$$

as $n \longrightarrow \infty$. To show that $\{\rho_n \circ \phi_{n,t}\}$ is $\rho(t)$-chaotic, it suffices to show that for all $k \in \mathbb{N}$,

$$\sum_{z_1,z_2,\dots,z_{n-k}\in\{1,2\}} \left[D_{\rho_n\circ\phi_{n,t}}\right]^{y_1,\dots,y_k,z_1,\dots,z_{n-k}}_{x_1,\dots,x_k,z_1,\dots,z_{n-k}} \longrightarrow \left[D_{\rho(t)}\right]^{y_1}_{x_1}\left[D_{\rho(t)}\right]^{y_2}_{x_2}\cdots\left[D_{\rho(t)}\right]^{y_k}_{x_k} \tag{13}$$

as $n \longrightarrow \infty$. We proceed to verify (13).

The operator $\mathcal{H}_n$ is diagonalized by the basis $\mathcal{E}_n$, and its diagonal entries are

$$[H_n]^{k_1,\dots,k_n}_{k_1,\dots,k_n} = \frac{1}{n}\sum_{r,s=1}^{n}\left(-J\eta(e_{k_r})\eta(e_{k_s}) - H\eta(e_{k_r})\right), \tag{14}$$

where

$$\eta(e_1) = +\frac{\hbar}{2}$$
$$\eta(e_2) = -\frac{\hbar}{2}.$$

Abbreviating $-J\eta(x)\eta(y) - H\eta(x)$ by $w(x,y)$, equations (9) and (14) imply that

$$[D_{\rho_n\circ\phi_{n,t}}]^{y_1,\dots,y_k,z_1,\dots,z_{n-k}}_{x_1,\dots,x_k,z_1,\dots,z_{n-k}} =$$
$$\exp\left(\frac{it}{\hbar n}\sum_{r,s=1}^{k}(w(y_r,y_s)-w(x_r,x_s))\right)\exp\left(H\frac{it}{\hbar}\frac{n-k}{n}\sum_{r=1}^{k}(\eta(x_r)-\eta(y_r))\right)\times$$
$$[D]^{y_1,\dots,y_k,z_1,\dots,z_{n-k}}_{x_1,\dots,x_k,z_1,\dots,z_{n-k}}\exp\left(J\frac{2it}{\hbar n}\sum_{r=1}^{k}\sum_{s=k+1}^{n}\eta(z_s)(\eta(x_r)-\eta(y_r))\right).$$

Therefore,

$$\begin{aligned}
&\lim_{n\to\infty}\sum_{z_1,\dots,z_{n-k}\in\{1,2\}}\left[D_{\rho_n\circ\phi_{n,t}}\right]^{y_1,\dots,y_k,z_1,\dots,z_{n-k}}_{x_1,\dots,x_k,z_1,\dots,z_{n-k}}\\
=\;&\exp\left(H\frac{it}{\hbar}\sum_{r=1}^{k}(\eta(x_r)-\eta(y_r))\right)\times\\
&\lim_{n\to\infty}\sum_{z_1,\dots,z_{n-k}\in\{0,1\}}[D]^{y_1,\dots,y_k,z_1,\dots,z_{n-k}}_{x_1,\dots,x_k,z_1,\dots,z_{n-k}}\exp\left(J\frac{2it}{\hbar n}\sum_{r=1}^{k}\sum_{s=k+1}^{n}\eta(z_s)(\eta(x_r)-\eta(y_r))\right)\\
=\;&\exp\left(H\frac{it}{\hbar}\sum_{r=1}^{k}(\eta(x_r)-\eta(y_r))\right)\times\\
&\lim_{n\to\infty}\sum_{z_1,\dots,z_{n-k}\in\{1,2\}}[D]^{y_1,\dots,y_k,z_1,\dots,z_{n-k}}_{x_1,\dots,x_k,z_1,\dots,z_{n-k}}\exp\left(J\frac{2it}{\hbar}\sum_{r=1}^{k}(\eta(x_r)-\eta(y_r))\frac{1}{n}\sum_{s=k+1}^{n}\eta(z_s)\right).
\end{aligned}$$

The last limit in the preceding equation may be calculated thanks to Lemma 1. To apply the lemma, fix $x_1, y_1, \dots, x_k, y_k \in \{1,2\}$ and define

$$f_n : \{1,2\} \longrightarrow \mathbb{C}; \qquad f_n(z_1,z_2,\dots,z_n) = [D]^{y_1,\dots,y_k,z_1,\dots,z_n}_{x_1,\dots,x_k,z_1,\dots,z_n}$$
$$G : [0,1] \longrightarrow \mathbb{C}; \qquad G(s) = \exp\left(Jit\sum_{r=1}^{k}(\eta(x_r)-\eta(y_r))(s-(1-s))\right).$$

The functions f_n are symmetric and satisfy condition (b) of the lemma, with

$$\begin{aligned} f(1) &= [D_\rho]_{e_1}^{e_1} \\ f(2) &= [D_\rho]_{e_2}^{e_2} \\ c &= [D_\rho]_{x_1}^{y_1} [D_\rho]_{x_2}^{y_2} \cdots [D_\rho]_{x_k}^{y_k} . \end{aligned}$$

The f_n also satisfy condition (a) of the lemma, for

$$\left| [D]_{x_1,\dots,x_k,z_1,\dots,z_n}^{y_1,\dots,y_k,z_1,\dots,z_n} \right| \leq \frac{1}{2} \left([D]_{x_1,\dots,x_k,z_1,\dots,z_n}^{x_1,\dots,x_k,z_1,\dots,z_n} + [D]_{y_1,\dots,y_k,z_1,\dots,z_n}^{y_1,\dots,y_k,z_1,\dots,z_n} \right)$$

by the positivity of D_{ρ_n}, so that

$$\sum_{z_1,\dots,z_{n-k}\in\{1,2\}} \left| [D]_{x_1,\dots,x_k,z_1,\dots,z_n}^{y_1,\dots,y_k,z_1,\dots,z_n} \right| \leq \operatorname{tr}(D_{\rho_n}) = 1.$$

Conclusion (i) of Lemma 1 now reveals that

$$\sum_{z_1,\dots,z_{n-k}\in\{1,2\}} [D]_{x_1,\dots,x_k,z_1,\dots,z_{n-k}}^{y_1,\dots,y_k,z_1,\dots,z_{n-k}} \exp\left(J \frac{2it}{\hbar} \sum_{r=1}^{k} (\eta(x_r) - \eta(y_r)) \frac{1}{n} \sum_{s=k+1}^{n} \eta(z_s) \right)$$

converges to

$$[D_\rho]_{x_1}^{y_1} [D_\rho]_{x_2}^{y_2} \cdots [D_\rho]_{x_k}^{y_k} \exp\left(Jit \left([D_\rho]_{e_1}^{e_1} - [D_\rho]_{e_2}^{e_2} \right) \sum_{r=1}^{k} (\eta(x_r) - \eta(y_r)) \right),$$

whence

$$\begin{aligned} & \lim_{n\to\infty} \sum_{z_1,\dots,z_{n-k}\in\{1,2\}} \left[D_{\rho_n \circ \phi_{n,t}} \right]_{x_1,\dots,x_k,z_1,\dots,z_{n-k}}^{y_1,\dots,y_k,z_1,\dots,z_{n-k}} \\ = \; & \exp\left(H \frac{it}{\hbar} \sum_{r=1}^{k} (\eta(x_r) - \eta(y_r)) \right) \times \\ & [D_\rho]_{x_1}^{y_1} [D_\rho]_{x_2}^{y_2} \cdots [D_\rho]_{x_k}^{y_k} \exp\left(Jit \left([D_\rho]_{e_1}^{e_1} - [D_\rho]_{e_2}^{e_2} \right) \sum_{r=1}^{k} (\eta(x_r) - \eta(y_r)) \right) \\ = \; & \prod_{r=1}^{k} [D_\rho]_{x_r}^{y_r} \exp\left\{ it \left(\eta(x_r) - \eta(y_r) \right) \left(H/\hbar + J \left([D_\rho]_{e_1}^{e_1} - [D_\rho]_{e_2}^{e_2} \right) \right) \right\} . \end{aligned}$$

This shows that $\{\rho_n \circ \phi_{n,t}\}$ is $\rho(t)$-chaotic, where

$$\left[D_{\rho(t)}\right]_x^y = [D_\rho]_x^y \exp\left\{it\left(\eta(x) - \eta(y)\right)\left(H/\hbar + J\left([D_\rho]_{e_1}^{e_1} - [D_\rho]_{e_2}^{e_2}\right)\right)\right\}.$$

Finally, it may be verified that the density operators $D_{\rho(t)}$ satisfy equation (8) of Conjecture 1.
■

4 Future Work

In future work, we hope to prove Conjecture 1, or at least to prove that the mean-field Heisenberg model propagates chaos. We shall also investigate the propagation of chaos by open systems (coupled to thermal baths) and prove the H-theorem for those processes.

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