5-1-1990

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Jian-Min Liu
University of Rhode Island

Gerhard Müller
University of Rhode Island, gmuller@uri.edu

Citation/Publisher Attribution

Jian-Min Liu, and Gerhard Müller. *The classical equivalent-neighbor XXZ model: exact results for dynamic correlation functions.* J. Appl. Phys. 67 (1990), 5489-5491.
Available at: http://dx.doi.org/10.1063/1.345860

The classical equivalent-neighbor *XXZ* model: Exact results for dynamic correlation functions

Jian-Min Liu and Gerhard Müller
Department of Physics, The University of Rhode Island, Kingston, Rhode Island 02881-0817

The dynamics of the classical XXZ model with uniform interaction is nonlinear for $N \geqslant 2$ spins and nonintegrable for $N \geqslant 3$. However, the nonlinearities disappear in the thermodynamic limit $N \to \infty$, and the spin autocorrelation functions can be determined exactly for infinite temperature. The function $\langle S_i^z(t) S_i^z \rangle$ exhibits a Gaussian decay to a nonzero constant, and the function $\langle S_i^x(t) S_i^x \rangle$ decays algebraically to zero or like a Gaussian, depending on the type (easy axis or easy plane) and amount of uniaxial anisotropy.

Equivalent-neighbor spin models consist of an array of N spins interacting via some model specific spin-pair interaction of uniform strength J'. Such models play a role in statistical mechanics of phase transitions as microscopic realizations of mean field theory.[1] In order to ensure that the free energy is an extensive quantity, the coupling strength must be scaled like $J' = J/N$. The consequence is that the system loses its intrinsic dynamics. For classical spins, this manifests itself in that the right-hand side of Hamilton's equation of motion for individual spins, $d\mathbf{S}_l/dt = -\mathbf{S}_l \times \partial H/\partial \mathbf{S}_l$, vanishes in the limit $N \to \infty$. For quantum spins, the same effect results from more subtle properties.[2]

However, a nontrivial dynamics (for $N \to \infty$) can be restored in equivalent-neighbor spin models if the spin coupling is scaled differently: $J' = J/\sqrt{N}$. The origin of these different scaling regimes is that the thermodynamic properties of the equivalent-neighbor model are governed by the mean value of the magnetization vector (which is the basis for Landau theory), while the dynamical properties are determined by the fluctuations about the mean value. A consistent description of dynamic correlation functions for equivalent-neighbor spin models in the canonical ensemble is then only possible at infinite temperature. Our dynamical study is thus strictly confined to the paramagnetic regime, specifically to $T = \infty$.

The classical equivalent-neighbor XXZ model is specified by the Hamiltonian

$$H = -\frac{1}{2\sqrt{N}} \sum_{\substack{ij=1 \\ i \neq j}}^{N} [J(S_i^x S_j^x + S_i^y S_j^y) + J_z S_i^z S_j^z]. \tag{1}$$

The equations of motion for classical spin variables $\mathbf{S}_i$ (three-component vectors of unit length) then read

$$\dot{S}_i^x = J_z \sigma_z S_i^y - J\sigma_y S_i^z - (1/\sqrt{N})(J_z S_i^z S_i^y - J S_i^y S_i^z), \tag{2a}$$

$$\dot{S}_i^y = J\sigma_x S_i^z - J_z \sigma_z S_i^x - (1/\sqrt{N})(J S_i^x S_i^z - J_z S_i^z S_i^x), \tag{2b}$$

$$\dot{S}_i^z = J(\sigma_y S_i^x - \sigma_x S_i^y), \tag{2c}$$

where the variable

$$\boldsymbol{\sigma} = \frac{1}{\sqrt{N}} \sum_{i=1}^{N} \mathbf{S}_i$$

represents the vector of instantaneous magnetization fluctuation. Given the fact (to be demonstrated later) that the length of $\boldsymbol{\sigma}$ is of $O(1)$, it follows that the $1/\sqrt{N}$ terms in Eqs. (2) become negligible in the thermodynamic limit. The dynamical problem then reduces to an effective two-spin model consisting of the collective spin $\boldsymbol{\sigma}$ and a single spin $\mathbf{S}_i$. The equations of motion for the collective spin variable σ_α,

$$\dot{\sigma}_x = (J_z - J)\sigma_z \sigma_y, \quad \dot{\sigma}_y = (J - J_z)\sigma_x \sigma_z, \quad \dot{\sigma}_z = 0,$$

obtained from summing Eqs. (2) over all sites i, dividing by $\sqrt{N}$, and taking the limit $N \to \infty$, prescribe a uniform precessional motion about the symmetry axis:

$$\sigma_x(t) = \sigma_\perp \cos(\Omega_z t + \phi_0),$$

$$\sigma_y(t) = \sigma_\perp \sin(\Omega_z t + \phi_0), \quad \sigma_z = \text{const},$$

with $\sigma_\perp^2 + \sigma_z^2 = \sigma^2 = \text{const}$ and precession frequency $\Omega_z = (J - J_z)\sigma_z$. For a given solution of $\boldsymbol{\sigma}(t)$, the equations of motion (2) for the individual spins $\mathbf{S}_i$ are then (for $N \to \infty$) linear first-order ODEs with time-periodic coefficients which are readily solved by standard methods:

$$\begin{aligned} S_i^x(t) = {} & \frac{1}{2} b_i \frac{\sigma_\perp}{\sigma + \sigma_z} \sin[(\bar{\Omega} + \Omega_z)t + \beta_i + \phi_0] \\ & - \frac{1}{2} b_i \frac{\sigma_\perp}{\sigma - \sigma_z} \sin[(\bar{\Omega} - \Omega_z)t + \beta_i - \phi_0] \\ & + z_i \frac{\sigma_\perp}{\sigma_z} \cos(\Omega_z t + \phi_0), \end{aligned} \tag{3a}$$

$$\begin{aligned} S_i^y(t) = {} & -\frac{1}{2} b_i \frac{\sigma_\perp}{\sigma + \sigma_z} \cos[(\bar{\Omega} + \Omega_z)t + \beta_i + \phi_0] \\ & - \frac{1}{2} b_i \frac{\sigma_\perp}{\sigma - \sigma_z} \cos[(\bar{\Omega} - \Omega_z)t + \beta_i - \phi_0] \\ & + z_i \frac{\sigma_\perp}{\sigma_z} \sin(\Omega_z t + \phi_0), \end{aligned} \tag{3b}$$

$$S_i^z(t) = b_i \sin(\bar{\Omega} t + \beta_i) + z_i, \tag{3c}$$

in terms of three integration constants z_i, b_i, β_i and the parameters of the driving field $\boldsymbol{\sigma}(t)$. The time evolution is harmonic, governed by two independent frequencies $\Omega_z = (J - J_z)\sigma_z$, $\bar{\Omega} = J\sigma$. Note, however, that for finite N, the $1/\sqrt{N}$ corrections in Eqs. (2) render the time evolution not only anharmonic but, in fact, nonintegrable, and are thus likely to ensure ergodicity and mixing.

0021-8979/90/095489-03$03.00

The single-spin autocorrelation functions $\langle S_i^\alpha(t) S_i^\alpha\rangle$ can then be evaluated by using the exact solutions (3) and performing the ensemble average in two steps. In the expressions

$$\langle S_i^x(t)S_i^x\rangle = \langle S_i^y(t)S_i^y\rangle$$

$$= \frac{1}{2}\left\langle z_i^2 \frac{\sigma^2 - \sigma_z^2}{\sigma_z^2}\cos(\Omega_z t)\right\rangle$$

$$+ \frac{1}{8}\left\langle b_i^2 \frac{\sigma - \sigma_z}{\sigma + \sigma_z}\cos[(\bar{\Omega} + \Omega_z)t]\right\rangle$$

$$+ \frac{1}{8}\left\langle b_i^2 \frac{\sigma + \sigma_z}{\sigma - \sigma_z}\cos[(\bar{\Omega} - \Omega_z)t]\right\rangle, \qquad (4a)$$

$$\langle S_i^z(t)S_i^z\rangle = \tfrac{1}{2}\langle b_i^2\cos(\bar{\Omega}t)\rangle + \langle z_i^2\rangle, \qquad (4b)$$

we have already performed a time average over one period of the closed orbit of the variable $\mathbf{S}_i(t)$. The remaining average over all initial conditions is complicated by the fact that the expressions on the right-hand side of (4) contain both local variables, z_i, b_i, and collective variables, σ, σ_z.

We can eliminate the local variables by exploiting the absence of any correlation between the instantaneous direction of a single spin and that of the collective spin: Express the integration constants z_i, b_i in terms of the initial conditions $S_i^\alpha(0)$ and use the result $\langle S_i^\alpha S_i^\beta f(\boldsymbol{\sigma})\rangle = (1/3)\langle f(\boldsymbol{\sigma})\rangle\delta_{\alpha\beta}$, which holds for an arbitrary function $f(\boldsymbol{\sigma})$, to obtain the relations

$$\langle z_i^2 f(\boldsymbol{\sigma})\rangle = \tfrac{1}{3}\langle(\sigma_z^2/\sigma^2) f(\boldsymbol{\sigma})\rangle,$$

$$\langle b_i^2 f(\boldsymbol{\sigma})\rangle = \tfrac{2}{3}\langle(1 - \sigma_z^2/\sigma^2) f(\boldsymbol{\sigma})\rangle.$$

We use these relations to derive from (4) expressions for $\langle S_i^\alpha(t)S_i^\alpha\rangle$ which are phase averages over functions that depend only on the collective variables σ, σ_z in addition to t:

$$\langle S_i^x(t)S_i^x\rangle = \frac{1}{6}\left\langle \frac{\sigma^2 - \sigma_z^2}{\sigma^2}\cos(\Omega_z t)\right\rangle$$

$$+ \frac{1}{6}\left\langle \frac{(\sigma - \sigma_z)^2}{\sigma^2}\cos[(\bar{\Omega} + \Omega_z)t]\right\rangle, \qquad (5a)$$

$$\langle S_i^z(t)S_i^z\rangle = \frac{1}{3}\left\langle \frac{\sigma^2 - \sigma_z^2}{\sigma^2}\cos(\bar{\Omega}t)\right\rangle + \frac{1}{3}\left\langle\frac{\sigma_z^2}{\sigma^2}\right\rangle. \qquad (5b)$$

For the evaluation of these expressions we need to know the joint probability distribution $P(\sigma, \sigma_z)$. The distribution function for the Cartesian components S_i^α of an individual spin is rectangular with variance 1/3:

$$P_1(S_i^\alpha) = \tfrac{1}{2}\Theta(1 - |S_i^\alpha|). \qquad (6)$$

In the absence of any instantaneous correlations between different spins, the central limit theorem implies that the collective spin variable is distributed according to a Gaussian distribution with the same variance:

$$P_\alpha(\sigma_\alpha) = C\exp(-3\sigma_\alpha^2/2), \quad C \equiv \sqrt{3/2\pi}.$$

The length of the vector $\boldsymbol{\sigma}$ is then characterized by a Maxwellian distribution

$$P(\sigma) = 4\pi C^3 \sigma^2 \exp(-3\sigma^2/2). \qquad (7)$$

Note that the collective spin has the same mean-square length, $\langle\sigma^2\rangle = 1$, as the single spin. The joint probability distribution $P(\sigma, \sigma_\alpha)$ can now be constructed from (7) and the conditional probability distribution [in generalization of (6)] $P(\sigma_\alpha|\sigma) = (1/2\sigma)\Theta(\sigma - |\sigma_\alpha|)$ via the relation $P(\sigma, \sigma_\alpha) = P(\sigma_\alpha|\sigma)P(\sigma)$ as

$$P(\sigma, \sigma_\alpha) = 2\pi C^3 \sigma\exp(-3\sigma^2/2)\Theta(\sigma - |\sigma_z|). \qquad (8)$$

This reduces the determination of the spin autocorrelation functions $\langle S_i^\alpha(t)S_i^\alpha\rangle$ or their spectral densities

$$\Phi_{\alpha\alpha}(\omega) = \int_{-\infty}^{+\infty} dt e^{i\omega t}\frac{\langle S_i^\alpha(t)S_i^\alpha\rangle}{\langle S_i^\alpha S_i^\alpha\rangle}$$

to the evaluation of elementary integrals. The results for the spectral densities are given by the following general closed-form expressions in terms of Gaussians, exponential integrals and error functions (for $J_\alpha \geqslant 0$):

$$\Phi_{xx}(\omega) = \frac{\pi^2 C^3}{|J - J_z|}\left\{\frac{2}{3}\exp\left(-\frac{3}{2}\frac{\omega^2}{(J - J_z)^2}\right) + \frac{\omega^2}{(J - J_z)^2}\mathrm{Ei}\left(-\frac{3}{2}\frac{\omega^2}{(J - J_z)^2}\right)\right.$$
$$+ \frac{1}{3}\frac{2J - J_z}{J - J_z}\left|\frac{2J - J_z}{J - J_z}\right|\left[\exp\left(-\frac{3}{2}\frac{\omega^2}{(2J - J_z)^2}\right) - \mathrm{sgn}(2J - J_z)\exp\left(-\frac{3}{2}\frac{\omega^2}{J_z^2}\right)\right]$$
$$- \frac{(2J - J_z)/C}{(J - J_z)|J - J_z|}|\omega|\left[\left|\mathrm{erf}\left(\sqrt{\frac{3}{2}}\frac{\omega}{J_z}\right)\right| - \left|\mathrm{erf}\left(\sqrt{\frac{3}{2}}\frac{\omega}{2J - J_z}\right)\right|\right]$$
$$\left.+ \frac{1}{2}\frac{\omega^2}{(J - J_z)|J - J_z|}\left[\mathrm{Ei}\left(-\frac{3}{2}\frac{\omega^2}{J_z^2}\right) - \mathrm{sgn}(2J - J_z)\mathrm{Ei}\left(-\frac{3}{2}\frac{\omega^2}{(2J - J_z)^2}\right)\right]\right\}, \qquad (9a)$$

$$\Phi_{zz}(\omega) = C^{\;\;2}\delta(\omega) + \frac{4\pi C\omega^2}{J^3}\exp\left(-\frac{3}{2}\frac{\omega^2}{J^2}\right). \qquad (9b)$$

We observe that the function $\Phi_{zz}(\omega)$ is independent of J_z, a peculiarity which is already present in the equation of motion (2c). The associated spin autocorrelation function,

$$3\langle S_i^z(t)S_i^z\rangle = \tfrac{1}{3} + \tfrac{2}{3}(1 - \tfrac{1}{3}J^2t^2)\exp(-J^2t^2/6),$$

decays like a Gaussian to a nonzero constant, 1/3. For the special case $J_z = J$, which represents the Kittel–Shore model, expression (9a) reduces to (9b). A special property of this model is that the time evolution is harmonic even for finite N.[3,4] The spectral density $\Phi_{xx}(\omega)$, by contrast, depends very sensitively on the uniaxial anisotropy. In the limiting case $J=0$, expression (9a) reduces to a simple Gaussian,

$$\Phi_{xx}(\omega) = (4\pi^2 C^3/3J_z)\exp(-3\omega^2/2J_z^2).$$

The associated correlation function is then also a Gaussian, $3\langle S_l^x(t)S_l^x\rangle = \exp(-J_z^2 t^2/6)$. As it turns out, the long-time asymptotic decay of $\langle S_l^x(t)S_l^x\rangle$ is Gaussian throughout the regime $J_z > 2J$ of easy-axis anisotropy. In the regime $0 < J_z < 2J$, $J_z \neq J$, the spectral density $\Phi_{xx}(\omega)$ has a singularity at $\omega = 0$ of the form $\Phi_{xx}(\omega) \sim \omega^2 \ln(\omega)$, which implies that the correlation function decays algebraically for long times, $\langle S_l^x(t)S_l^x\rangle \sim t^{-3}$. In the limit $J_z = 0$, a stronger singularity in the spectral density makes its appearance, $\Phi_{xx}(\omega) \sim |\omega|$, implying a slower long-time asymptotic decay of the associated correlation function, $\langle S_l^x(t)S_l^x\rangle \sim t^{-2}$.

Some time ago, Lee, Dekeyser, and Kim[5-7] studied the dynamical properties of the quantum spin-1/2 equivalent-neighbor XXZ model, using quite different calculational techniques. Their analysis of the spin autocorrelation functions is not as complete as the one presented here for the classical model, but they found essentially the same long-time asymptotic behavior of the function $\langle S_l^x(t)S_l^x\rangle$.[7] We can in fact prove that quantum effects are completely negligible in the dynamics of equivalent-neighbor spin models.[2] A study of the more general equivalent-neighbor XYZ model is currently in progress. The $T=\infty$ dynamics of that model can also be mapped onto an effective two-body problem, but one with nonlinear time evolution. Not surprisingly, these anharmonicities add a considerable amount of complexity to the structure of the dynamic correlation functions.

This work was supported in part by the U.S. National Science Foundation Grant No. DMR-86-03036.

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