Time-Dependent Behavior of the Spin-$\frac{1}{2}$ Anisotropic Heisenberg Model in Infinite Lattice Dimensions

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The spin van der Waals model may be regarded as an infinite-lattice-dimensional limit of the spin-$\frac{1}{2}$ anisotropic Heisenberg model. By solution of the generalized Langevin equation, time-dependent behavior is obtained. The geometry of realized Hilbert spaces lends a simple interpretation for critical dynamics.

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Certain statistical mechanical models are exactly solvable at some special limits, providing useful insight into the behavior of these models. For example, when the spin dimensionality in the classical Heisenberg model is made infinitely large, one obtains the spherical model.[1] The static behavior of this model is well understood[2] and has been useful for understanding critical behavior.[1]

Consider the spin-$\frac{1}{2}$ nearest-neighbor (nn) anisotropic Heisenberg model on a hypercubic lattice of dimensionality D,

$$H = -\sum_{\alpha}\sum_{(i,j)} J_{ij}^{\alpha}(D) s_i^{\alpha} s_j^{\alpha}, \tag{1}$$

where $\alpha = x,y,z$. An infinite-*lattice*-dimensional limit[3] ($D \to \infty$) of (1) is the spin van der Waals model.[4] Statically this limit is uninteresting since the model should behave in a mean-field fashion. However, it may qualitatively describe the time-dependent behavior of the quantum model in finite lattice dimensions. Other than in $D=1$ at $T=0$ or $T\to\infty$, the time-dependent behavior of (1) is not exactly known presently. We provide here the nonequilibrium behavior of the spin van der Waals model by solving the generalized Langevin equation.

The problem of time evolution in (1) for, e.g., the total spin $S_\alpha = \sum_{i=1}^{N} s_i^{\alpha}$ is defined by the generalized Langevin equation:

$$dS_\alpha(t)/dt + \int_0^t dt'\, \phi_\alpha(t-t') S_\alpha(t') = F_\alpha(t),$$

where F_α and ϕ_α are, respectively, the random force and memory function. According to the method of recurrence relations[5] one constructs a d-dimensional Hilbert space $\mathscr{S}_0^{(d)}$ for S_α spanned by orthogonal basis vectors of $f_0, f_1, \ldots, f_{d-1}$. For statistical mechanical problems generally, $\mathscr{S}_0^{(d)}$ is realized by the inner product,

$$(X,Y) = \beta^{-1}\int_0^{\beta} d\lambda\, \langle e^{\lambda H} X e^{-\lambda H} Y\rangle - \langle X\rangle\langle Y\rangle,$$

for X and $Y \subset \mathscr{S}_0^{(d)}$, where $\beta = 1/kT$, $\langle XY\rangle = \mathrm{Tr}(XYe^{-\beta H})/\mathrm{Tr}(e^{-\beta H})$. The orthogonal basis vectors for this space have the property that they are connected by a recurrence relation[5]

$$f_{\nu+1} = \dot{f}_\nu + \Delta_\nu f_{\nu-1}, \tag{2}$$

where $\dot{f}_\nu = i[H, f_\nu]$ and $\Delta_\nu = (f_\nu, f_\nu)/(f_{\nu-1}, f_{\nu-1})$, referred to as the νth recurrant. Then $S_\alpha(t) = \sum_{\nu=0}^{d-1} a_\nu(t) f_\nu$, $F_\alpha(t) = \sum_{\nu=1}^{d-1} b_\nu(t) f_\nu$, $\phi_\alpha(t) = \Delta_1 b_1(t)$, where a_ν's and b_ν's are autocorrelation functions describing relaxation and memory, respectively. The two families are related by a convolution $a_\nu(t) = \mathrm{conv.}\{a_0(t) * b_\nu(t)\}$, $\nu \geq 1$. Both functions must satisfy an identical recurrence relation, e.g.,

$$\Delta_{\nu+1} a_{\nu+1}(t) = -\dot{a}_\nu(t) + a_{\nu-1}(t), \tag{3}$$

where $\dot{a}_\nu = da_\nu(t)/dt$, $0 \leq \nu \leq d-1$.

We take the limit $D\to\infty$ in (1), i.e., the spin van der Waals model form with $J_{ij}^{x}(D) = J_{ij}^{y}(D) = J/N$ and $J_{ij}^{z}(D) = J_z/N$, where J and J_z are nonnegative. Then for $f_0 = S_x$, i.e., $\alpha = x$, we obtain, using (2),

$$f_1 = -2\omega S_z S_y, \quad f_2 = -4\omega^2 S_z^2 S_x + \Delta_1 S_x,$$
$$f_3 = 8\omega^3 S_z^3 S_y - 2(\Delta_2 + \Delta_1)\omega S_z S_y,$$
$$f_4 = 16\omega^4 S_z^4 S_x - 4(\Delta_3 + \Delta_2 + \Delta_1)\omega^2 S_z^2 S_x + \Delta_3 \Delta_1 S_x,$$

etc.,[6] where $\omega = (J - J_z)/N$ and $\hbar \equiv 1$.

To evaluate the norm (f_ν, f_ν) of f_ν explicitly, one needs to know the ensemble averages of spins which appear in the inner product.[5] Thus the evaluation depends on whether $J > J_z$ (XY regime) or $J < J_z$ (Ising regime) and also whether $T > T_c$ (high temperature) or $T < T_c$ (low temperature).

XY regime.—For $T > T_c = J/2k$, it was shown[7] that

$$\langle S_z^{2\nu} S_x^2 \rangle = \langle S_z^{2\nu} \rangle \langle S_x^2 \rangle,$$
$$\langle S_z^{2\nu} \rangle = (2\nu - 1)!! \langle S_z^2 \rangle^\nu, \qquad \nu = 1, 2, 3, \ldots,$$

where $\langle S_z^2 \rangle = \frac{1}{2}N/(2 - \beta J_z)$ and $\langle S_x^2 \rangle = \frac{1}{2}N/(2 - \beta J)$. Using these results and retaining only the leading terms of N, we obtain $(f_\nu, f_\nu) = \langle S_x^2 \rangle$.[7] Hence the νth recurrant is $\Delta_\nu = \nu(4\omega^2 \langle S_z^2 \rangle) \equiv \nu\Delta$, $\nu \geq 1$. The upper limit on ν is unbounded. Hence $d \rightarrow \infty$.

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For $T < T_c$, there now exists an ordered phase, i.e, $\langle S_x \rangle = O(N)$.[4] However, the same form of decoupling is still valid provided that one substitutes $\langle S_z^2 \rangle = \frac{1}{2}N/\beta(J - J_z)$ and $\chi = \langle S_x^2 \rangle - \langle S_x \rangle^2$. Thus the norm of f_ν for $T < T_c$ has the same form and the structure of recurrants is consequently identical whether T is above or below T_c.

Ising regime.—For $T > T_c = J_z/2k$ the Ising and XY static properties are identical.[7] Hence one also has $\Delta_\nu = \nu\Delta$ for the high-temperature Ising regime.

For $T < T_c$ the ordered phase is characterized by $\langle S_z \rangle = O(N)$.[4] Although still $\langle S_z^{2\nu} S_x^2 \rangle = \langle S_z^{2\nu} \rangle \times \langle S_x^2 \rangle$, one now has[4] $\langle S_z^{2\nu} \rangle = \langle S_z \rangle^{2\nu}$. Using it, we find that $(f_0, f_0) = \chi$ and $(f_1, f_1) = 4\omega^2 \langle S_z \rangle^2 \chi$. Hence $\Delta_1 = 4\omega^2 \langle S_z \rangle^2 \equiv \Omega^2$. Using these results, we see that $(f_2, f_2) = 0$. Hence also $\Delta_2 = 0$. A more careful analysis shows that $(f_\nu, f_\nu) = O(N)$ if $\nu = 0$ and 1, but $(f_\nu, f_\nu) = O(N^{-1})$ if $\nu \geq 2$. This behavior of the basis vectors implies that the d-dimensional Hilbert space $\mathscr{S}_0^{(d)}$ becomes effectively reduced to a two-dimensional space, i.e., $\mathscr{S}_0^{(d)} = \mathscr{S}_0^{(d)} \otimes \mathscr{S}_2^{(d-2)}$, where $\mathscr{S}_0^{(2)}$ is a two-dimensional (2D) space spanned by f_0 and f_1, and $\mathscr{S}_2^{(d-2)}$ is a $(d-2)$-dimensional subspace spanned by $f_2, \ldots, f_{d-1}$. The time evolution of S_x is confined to the 2D space $S_0^{(2)}$ at all times. It does not extend into the subspace $\mathscr{S}_2^{(d-2)}$. In this 2D space there is only one recurrant, $\Delta_1 = \Omega^2$. This is in contrast to the high-temperature Ising regime, where the time evolution of S_x extends into an infinite-dimensional space.

Given the structure of recurrants, the recurrence relation (3) can now be realized. For the XY and high-temperature Ising regimes, we have

$$(\nu + 1)\Delta a_{\nu+1}(t) = -\dot{a}_\nu(t) + a_{\nu-1}(t), \qquad (4)$$

$0 \leq \nu \leq \infty$. The recurrence relation is satisfied by

$$a_\nu(t)(t^\nu/\nu!)\exp(-\tfrac{1}{2}\Delta t^2), \qquad (5)$$

where $\Delta^{1/2}$ will be referred to as the *basal frequency*. Using (5) we can now obtain b_ν by solving the convolution equation for b_ν.

For the low-temperature Ising regime, $d = 2$ and $\Delta_1 = \Omega^2$ only. Thus, the recurrence relation (3) assumes $\dot{a}_1(t) = a_0(t)$, $\Omega^2 a_1(t) = -\dot{a}_0(t)$. Hence $a_0(t) = \cos\Omega t$, $a_1(t) = \sin\Omega t/\Omega$, where Ω is now the basal frequency. From the convolution equation, we have $b_1(t) = 1$ for all times.

Viewing through the realized Hilbert spaces, we see that the time evolution of S_x traces a trajectory. In the XY and high-temperature Ising regimes, the trajectory is spirallike, starting from the basal vector f_0 and winding towards the highest vector $f_{d\rightarrow\infty}$. In the low-temperature Ising regime, the trajectory can only be rotational, being confined to a two-dimensional space. These trajectories can be regarded as being drawn out by the random force which may itself evolve in time. In the XY and high-temperature Ising regimes, the trajectory of the random force is also spirallike, starting off at f_1. Hence it continuously draws S_x into higher reaches of the Hilbert space. In the low-temperature Ising regime, the random force lies in a one-dimensional manifold and is stationary at f_1. As a result, S_x is not pulled out of its two-dimensional confine.

In Figs. 1 and 2 we illustrate the a_ν's and b_ν's for the XY and high-temperature Ising regimes as functions of time. The temperature and interaction symmetry enter into these autocorrelation functions through the basal frequency $\Delta^{1/2} = 2|\omega| \langle S_z^2 \rangle^{1/2}$. What is shown in, e.g., Fig. 1 is the distribution of projections of $S_x(t)$ onto various basis vectors. The distribution rapidly shifts with time from the basal vector towards higher vectors. The random force appears to have a similar distribution, indicating that on the high-temperature side there is but one time scale in the system. In Brownian theories it is usually assumed that there are two distinct time scales, one for the relaxation functions, a_ν's, and

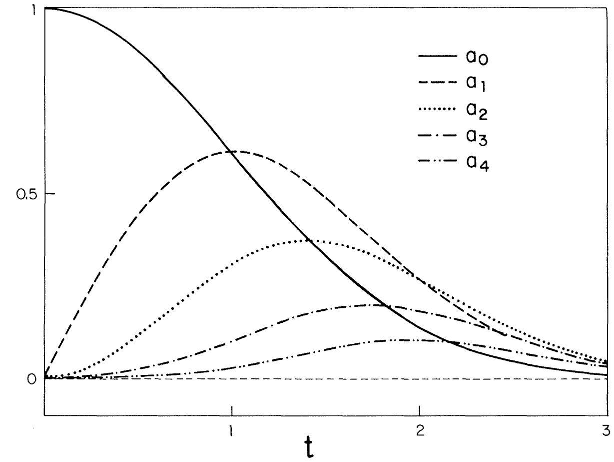

FIG. 1. Relaxation functions $a_\nu(t)$ vs time at $T > T_c$ in the XY and Ising regimes. The time is given in units of $\Delta^{1/2} = 2|\omega|\langle S_z^2\rangle^{1/2}$. $a_0(t) = (S_x(t),S_x)/(S_x,S_x)$, $a_1(t) = (S_x(t),\dot{S}_x)/(\dot{S}_x,\dot{S}_x)$, etc.

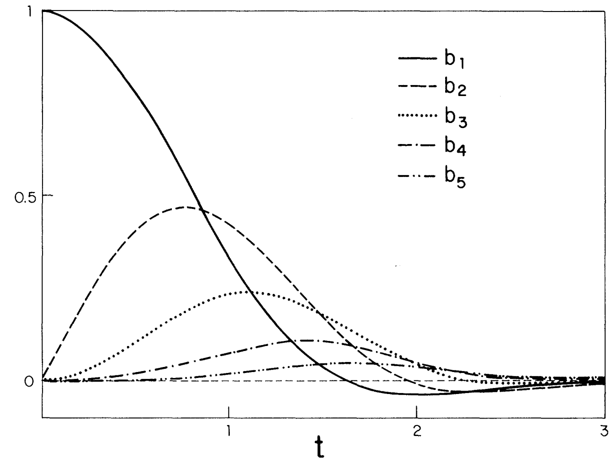

FIG. 2. Memory functions $b_\nu(t)$ vs time at $T > T_c$ in the XY and Ising regimes. The time is given in units of $\Delta^{1/2}$. $b_\nu(t)$'s are related to $a_\nu(t)$'s via a convolution: $a_\nu(t) = \int_0^t dt'\, a_0(t-t')b_\nu(t')$, $\nu \geq 1$.

another for the memory functions, b_ν's.[8]

In Fig. 3, the spin-velocity autocorrelation function $\dot{a}_1$ is compared with a_0 and b_1. The behavior of a_0 and $\dot{a}_1$ is strikingly similar to what Windsor found by computer simulation for the simple-cubic, nearest-neighbor classical Heisenberg model at high temperatures.[9] Also our result for a_0 resembles the computer-simulated long-wavelength high-temperature relaxation function for the one-dimensional Heisenberg model.[10] The resemblance suggests that high-temperature spin dynamics is not overly sensitive to the large-dimensional limit that we have taken.

The behavior of the basal frequency as $T \rightarrow T_c$ determines the nature of critical dynamics. Critical anomalies are indicated by accompanying changes in the structure of the Hilbert space $\mathscr{S}_0^{(d)}$. For the XY regimes, the basal frequency is $\Delta^{1/2} = 2|\omega|\langle S_z^2\rangle^{1/2}$, where $\langle S_z^2\rangle = \frac{1}{2}N/(2-\beta J_z)$ for $T > T_c$ and $\langle S_z^2\rangle = \frac{1}{2}N/\beta(J-J_z)$ for $T < T_c$. Since $J > J_z$ and $\beta_c J = 2$ for the XY regime, the basal frequency remains finite as T approaches T_c from above or below. Thus there is no critical anomaly associated with the time evolution of S_x in the XY regime. The structure of $\mathscr{S}_0^{(d)}$ is unaffected by T crossing T_c.

For the high-temperature Ising regime, the basal frequency is the same as that for the high-temperature XY regime, but it can now diverge because $\beta_c J_z = 2$. Hence as $T \rightarrow T_c^+$, the trajectory spirals more quickly towards higher dimensions in an infinite-dimensional space. For $T < T_c$ the basal frequency is $\Omega = 2|\omega|\langle S_z\rangle$, which vanishes as $T \rightarrow T_c^-$. Thus the rotational trajectory in a two-dimensional space is slowed down as $T \rightarrow T_c^-$. The time evolution appears to show two types of critical dynamics. What is evidently being manifested is that the two sides of T_c enjoy vastly different time scales. On the high-temperature side, the time scale is of order $N^{1/2}$,[11] whereas on the low-temperature side it is $O(1)$. As, e.g., $T \rightarrow T_c^+$, the two time scales must match up at T_c. They apparently do so by speeding up of the spiraling trajectory. In the process the spiral forming in an

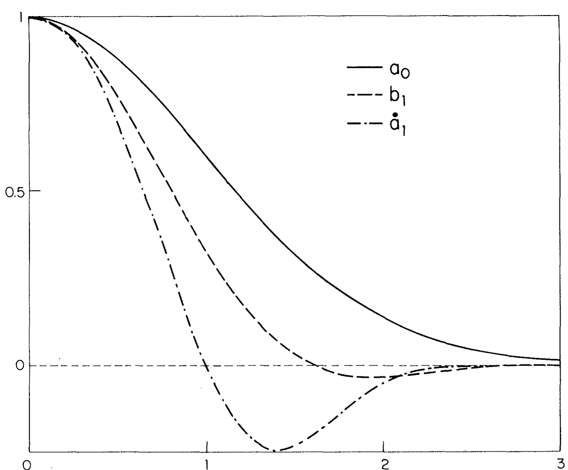

FIG. 3. Spin-velocity autocorrelation function $\dot{a}_1(t)$ compared with $a_0(t)$ and $b_1(t)$ at $T > T_c$ in the XY and Ising regimes. The time is given in units of $\Delta^{1/2}$. $\dot{a}_1(t) = (\dot{S}_x(t),\dot{S}_x)/(\dot{S}_x,\dot{S}_x)$.

infinite-dimensional space "tumbles" over into a two-dimensional space as T crosses T_c from above.

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