Conserved Ordering Dynamics of Heisenberg Spins with Torque

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We show that a torque induced by the local molecular field drives the zero-temperature ordering dynamics of a conserved Heisenberg magnet to a new fixed point, characterised by exponents $z = 2$ and $\lambda \approx 5.15$. Numerical solutions of the Langevin equation indicate that theories using a Gaussian closure are inconsistent even when the torque is absent. The torque is relevant even for quenches to $T_c$, with exponents $z = 4 - \varepsilon/2$ and $\lambda = d$ (where $\varepsilon = 6 - d$). Indeed $\lambda$ is always equal to $d$ for quenches to $T_c$ whenever the order parameter is conserved.

When a magnet is quenched from its disordered high temperature phase to its ordered configuration at low temperatures, the slow annealing of "defects" separating competing domains, makes the dynamics very slow. The system organizes itself into a self similar spatial distribution of domains characterised by a single diverging length scale which typically grows algebraically in time $L(t) \sim t^{1/2}$. This spatial distribution of domains is reflected in the scaling behaviour of the equal-time correlation function $C(r, t) \sim f(r/L(t))$. The autocorrelation function, $C(0, 0; 0, t) \sim L(t)^{-\lambda}$ is a measure of the memory of the initial configurations. The exponents $z$ and $\lambda$ and the scaling function $f(x)$ characterise the dynamical universality classes at the zero temperature fixed point (ZFP).

There has been a trend in recent years to compare the theories of phase ordering dynamics with numerical simulations of Langevin equations. Comparison with experimental systems, such as magnets, binary fluids or binary alloys have to take into account the various "real" features that might be relevant to its late time dynamics. For instance, theories of binary fluids have to include effects of hydrodynamics, while those of binary alloys have to incorporate elastic and hydrodynamic effects. In the same vein, any comparison with the dynamics in real magnets has to include the effects of the torque induced by the local molecular field.

In this article, we study the conserved phase ordering dynamics of a Heisenberg magnet in three dimensions in the presence of a torque (the corresponding nonconserved dynamics has been studied in Ref. [2]). For quenches to $T = 0$, our Langevin simulation conclusively shows that the torque drives the dynamics to a new ZFP characterised by $z = 2$ and $\lambda \approx 5.15$. This is confirmed by simple scaling arguments, which in addition gives the crossover time and the crossover exponent. Further we demonstrate that the approximate theories of conserved dynamics for vector order parameters based on the Gaussian closure scheme [4], are internally inconsistent even when the torque is absent, contrary to what has been assumed in the literature [3].

We investigate the dynamics following a quench to the critical point $T_c$ and show that the torque is relevant at the Wilson-Fisher fixed point. Using a diagrammatic perturbation theory, we show that $z = 4 - \varepsilon/2$ at this new fixed point (where $\varepsilon = 6 - d$). We show to all orders in a perturbative expansion, that the autocorrelation exponent $\lambda = d$. This last result is true whenever the order parameter is conserved and can be understood from very general arguments [2].

The Heisenberg model in 3-dim is described by a vector order parameter $\vec{\phi}(r, t)$ and a free-energy functional,

$$ F[\vec{\phi}] = \int d\mathbf{r} \left[ \frac{1}{2} \left( \nabla \vec{\phi} \right)^2 + \frac{\mu}{2} \vec{\phi} \cdot \vec{\phi} + \frac{u}{4} \left( \vec{\phi} \cdot \vec{\phi} \right)^2 \right]. \quad (1) $$

This leads to the following dynamical equation (in dimensionless quantities), describing zero temperature quenches of the conserved Heisenberg model [2],

$$ \frac{\partial \vec{\phi}}{\partial t} = \nabla^2 \left( \nabla^2 \vec{\phi} + \vec{\phi} - \left( \vec{\phi} \cdot \vec{\phi} \right) \vec{\phi} \right) + g \left( \vec{\phi} \times \nabla^2 \vec{\phi} \right). \quad (2) $$

The first term on the right side is the dissipative force, while the second term is the torque generated by the local molecular field. The dimensionless parameter $g \sim \Omega / T$ is the ratio of the precession frequency to the relaxation rate and is in the range $10^{-3} - 10$ for real magnets.

We discretize Eq. (2) on a simple cubic lattice (with size $N$ ranging from $30^3$ to $60^3$) adopting an Euler scheme for the derivatives. We include the next-nearest neighbour contributions in calculating the second and higher order spatial derivatives which reduces lattice anisotropy and gives better numerical stability [3]. The space and time intervals have been chosen to be $\Delta x = 2.5$ and $\Delta t = 0.2$ which lead to stable results for the resulting coupled map. We have checked that slight variations of $\Delta x$ and $\Delta t$ do not change the results. Throughout our simulation we have used periodic boundary conditions. We prepare the system initially in the paramagnetic phase, where $\vec{\phi}$ is distributed uniformly with zero mean (angular brackets denote an average over this distribution).

In our simulations we find that averaging over 5 initial uncorrelated configurations

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gives us clean results (the statistical errors in $C(r, t)$ are at most 3%).

We compute the equal-time correlator $C(r, t) \equiv \langle \bar{\phi}(r, t) \cdot \bar{\phi}(0, t) \rangle$, the autocorrelation function, $C(0, t_1 = 0, t_2) \equiv \langle \bar{\phi}(0, 0) \cdot \bar{\phi}(0, t_2) \rangle$ and the energy density. Figure 1 is a scaling plot of $C(r, t)$ versus $r/L(t)$ for various values of the parameter $g$, where $L(t)$ is extracted from the first zero of $C(r, t)$. Note that the scaling function for $g = 0$ is very different from those for $g > 0$; further the $g > 0$ scaling functions do not seem to depend on the value of $g$. This suggests that the torque term drives the dynamics to a new ZFP. This is also revealed in the values of the dynamical exponent $z$. In Fig. 2, a plot of $L(t)$ versus $t$ gives the expected value of $z = 4$ when $g = 0$. For $g > 0$, we see a distinct crossover from $z = 4$ when $t < t_c(g)$ to $z = 2$ when $t > t_c(g)$. The crossover time $t_c(g)$ decreases with increasing $g$. The same $z$ exponent and crossover are obtained from the scaling behaviour of the energy density, $\varepsilon = \frac{1}{t} \int dr \langle (\nabla \bar{\phi}(r, t))^2 \rangle \sim L(t)^{-2}$.

We provide a simple scaling argument to understand some of the results quoted above. On restoring appropriate dimensions, the dynamical equation Eq. (3) can be rewritten as a continuity equation, $\partial \bar{\phi}(r, t)/\partial t = -\nabla \cdot \vec{j}$ where the “spin current”

$$\vec{j}_\alpha = -\Gamma \left( \frac{\nabla F[\bar{\phi}]}{\delta \phi_\alpha} + \frac{\Omega}{M} \epsilon_{\alpha\beta\gamma} \phi_\beta \nabla \phi_\gamma \right). \tag{3}$$

Using a dimensional analysis where we replace $j_\alpha$ by the ‘velocity’ $dL/dt$, we find

$$\frac{dL}{dt} = \frac{\sigma}{L^3} + \frac{\Omega M_0}{L}, \tag{4}$$

where $M_0$, $\sigma$ and $\Gamma^{-1}$ are the equilibrium magnetisation, surface tension and spin mobility respectively. Beyond a crossover time given by $t_c(g) \sim (\Gamma/M_0 \Omega)^2 \sim 1/g^2$, simple dimension counting shows that the dynamics crosses over from $z = 4$ to $z = 2$ in conformity with our numerical simulation.

The $g$ dependence of the crossover time $t_c$ is also borne out by our numerics (Fig. 2 (inset)) as we demonstrate below. Equation (4) suggests the scaling ansatz $L(t, g) = t^{s(g)}$ valid for all $g$. This scaling form is governed by the $g = 0$ ZFP, and so the scaling function $s(x)$ should asymptote to a $g$-independent constant $s_0$ as $x \to 0$. This implies that $\alpha = 1/4$. On the other hand, as $x \to \infty$, $s(x) \sim x^{1/4}$. If the above proposal is true, then the data for $L(t, g)/t^{1/4}$ versus $tg^2$ should collapse onto a scaling
curve for an appropriate value of $\phi$. We find that $\phi \approx 1.7$. Thus the crossover time, obtained when $tg^0 = 1$, goes as $t_c \sim g^{-1.7}$, close to our earlier estimate. Note that our numerical estimate of the crossover exponent can be improved by introducing finite-time shift factors.

Can the above results be understood within the class of approximate theories based on the gaussian closure approximation [4]? The gaussian closure method consists of trading the order parameter $\tilde{\phi}(r, t)$ which is singular at defect sites, for an everywhere smooth field $m(r, t)$, defined by a nonlinear transformation, $\tilde{\phi}(r, t) = \sigma(m(r, t))$. Correlation functions are calculated making the single assumption that each component of $m(r, t)$ is an independent gaussian field with zero mean at all times. The equal time correlation function takes the form [6]

$$C(r, t) = \frac{3\gamma}{2\pi} \left[ B \left( \frac{2}{4}, \frac{1}{4} \right) \right]^2 2F_1 \left( \frac{1}{4}, \frac{1}{4}, \frac{3}{2}; \gamma^2 \right)$$

where $B(x, y)$ and $2F_1(a, b, c; z)$ are the Beta and hypergeometric functions respectively and $\gamma(r, t) = \langle m(m + x, t) \cdot m(x, t)^2 \rangle$. This scheme which works remarkably well for nonconserved systems [3] fails to give consistent results for our conserved dynamics, as we show, using a criterion developed by Yeung et. al. [7].

We numerically evaluate the spectral density, the fourier transform of $\gamma(r, t)$. This is prone to numerical errors because of statistical errors in our computed $C(r, t)$. For instance, a numerical integration of $\int dr C(r, t)$ provides a nonzero value whereas it should be identically zero because of the conservation law. This is reflected in large errors in $\gamma(k, t)$ at small $k$. We therefore adopt the following procedure. We fit a function $C_f(x)$ [3] to the equal time correlation function $C(r, t)$ and use this to extract $\gamma(k, t)$ from the Eq$(5)$. We observe (Fig.3) that the spectral density, which should be a strictly positive function of its arguments, becomes negative for $k/k_m < 0.5 \ (\gamma(k, t)$ is peaked at $k_m)$ and in the range $1.5 < k/k_m < 3.0$! This demonstration highlights the intrinsic inconsistency of the gaussian approach for conserved vector order parameters.

We investigate the dynamics of the order parameter quenched to the critical point $T_c$. At the Wilson-Fisher fixed point, $u^* = (8/11)\pi^2 \epsilon$ ($\epsilon = 4 - d$), the scaling dimension of $g$ is $d/2 + 1 - z + \eta/2$, where $z = 4 - \eta$ and $\eta = (5/24)(2\epsilon)$ implying that the torque $g$ is relevant when $d < 6$.

We calculate the dynamical exponents $z$ and $\lambda$ at this new fixed point. This is done using a diagrammatic perturbation theory within the Martin-Siggia-Rose (MSR) formalism [8]. For our problem, the MSR generating functional is, $Z[\bar{h}, \bar{h}] = \int D(\bar{\phi})D(\bar{\phi}) \exp (-J[\bar{\phi}, \bar{\phi}] - H_0[\phi(0)] + \int_0^\infty dt \int d\k \tilde{h}_\k \cdot \tilde{\phi}_\k + \tilde{h}_\k \cdot \tilde{\phi}_{-\k})$ where the MSR action is

$$J[\bar{\phi}, \bar{\phi}] = \int_0^\infty dt \int d\k \left\{ \frac{\sigma^2}{2} \left[ \partial_t \phi_\k + \Gamma k^2 \delta F[\phi] \right] \right\}$$

$$+ \int d\k \left( \frac{g^2}{2} (k^2 - (k - k_1)^2) \tilde{\phi}_\k \cdot \tilde{\phi}_{-\k} \right)$$

and $H_0$ denotes initial distribution (gaussian with width $\tau_0^{-1}$ and spatially uncorrelated) of the order parameter $H_0 = \int d\k \tilde{\phi}_\k(0) \cdot \tilde{\phi}_{-\k}(0)$ [3].

Power counting reveals the presence of two different upper critical dimensions coming from the quartic term ($d^2l^2 = 4$) and the cubic torque term ($d^2l^2 = 6$) in the action $J$. This implies we have to evaluate the fixed points and exponents in a double power series expansion in $\epsilon = 4 - d$ and $\epsilon = 6 - d$ [3].

The unperturbed correlation $C^0_k(t_1, t_2)$ and response $G_k^0(t_1, t_2)$ functions, and the bare $u$ and $g$ vertices are shown in Fig. 4. Again power counting shows that at $d = 3$, our perturbation expansion does not generate additional terms other than those already contained in $J$, i.e. the theory is renormalizable. However the perturbation theory gives rise to ultraviolet divergences which can be removed by adding counter-terms to the action.

To remove these divergences, we introduce renormalization factors (superscripts $R$ and $B$ denote renormalized and bare quantities respectively), $\tilde{\phi}^R_k(t) = (Z_0)^{-1/2} \tilde{\phi}^B_k(t)$, $\phi^R_k(t) = Z^{-1/2} \phi^B_k(t)$, $\phi^R_k(t) = Z^{-1/2} \phi^B_k(t)$, $u^R = Z_u^{-1} u^B$, $g^R = Z_g^{-1} g^B$, $\Gamma^R = Z_t^{-1} \Gamma^B$ and $\tau_0^R = Z_{\tau_0}^{-1} \tau_0^B$.

Since the dynamics obeys detailed balance, the renormalization factors $Z$ and $Z_u$ are the same as in statics.
Further the conservation of the order parameter forces $ZZ = 1$ to all orders.

The new fixed point is given by the zeroes of the β functions of the theory. The β functions, calculated from the Z factors, get contributions from all diagrams containing the primitively divergent diagrams $\Gamma^{(2)}_{\phi\phi}$, $\Gamma^{(3)}_{\phi\phi\phi}$ and $\Gamma^{(4)}_{\phi\phi\phi\phi}$ (Fig. 4).

The new fixed point, to one loop, is given by

$$\lambda \approx 4 - \varepsilon/2 + O(\varepsilon^2)$$

(4)

This implies that $G^B_k(t,0)$ does not get renormalized and $Z_0 = 1$. Consequently λ stays at its mean-field value of $d$ for this conserved Heisenberg dynamics both with and without the torque $T$.

We have shown that the inclusion of a torque to the ordering dynamics of a conserved Heisenberg magnet, is relevant both for quenches to $T = 0$ and $T > T_c$. The new zero temperature fixed point is characterised by exponents $z = 2$ and $\lambda \approx 5.15$. We have provided scaling arguments to understand these exponents and the crossover. We have shown that the class of approximate theories based on the Gaussian closure scheme which had been constructed to understand this zero temperature conserved dynamics, are inconsistent even when the torque is absent. On the other hand, the new critical fixed point is characterised by exponents $z = 4 - \varepsilon/2$ and $\lambda = d$ (where $\varepsilon = 6 - d$). Indeed λ is always equal to $d$ for quenches to the critical point whenever the order parameter is conserved.

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\[\text{FIG. 4. Unperturbed (a) response function } G^0_{k}(t) \text{, (b) correlation function } C^0_{k}(t) \text{, and the (c) two bare vertices } u \text{ and } g. \text{ Wavy and straight lines represent the } \tilde{\phi}_k(t) \text{ and } \tilde{\phi}_k(t) \text{ fields respectively. (d) Primitively divergent diagrams } \Gamma^{(2)}_{\phi\phi}, \Gamma^{(3)}_{\phi\phi\phi} \text{ and } \Gamma^{(4)}_{\phi\phi\phi\phi}.\]

The λ exponent can be computed from the response function $G_{k}(t,0) \equiv \langle \tilde{\phi}_k(0) \cdot \tilde{\phi}_{-k}(t) \rangle$ since this is equal to the autocorrelation function $\tau_0^{-1} \langle \tilde{\phi}_{k}(t) \cdot \tilde{\phi}_{-k}(0) \rangle$, as can be seen from the first term in $J$ by integrating by parts. The response function gets renormalized by

$$G^R_k(t,0) = Z_0^{-1/2}G^B_k(t,0). \tag{7}$$

The divergent contributions to $G_B$ could come from two sources. Each term in the double perturbation series could contain the primitively divergent subdiagrams $\Gamma^{(2)}$, $\Gamma^{(3)}$ or $\Gamma^{(4)}$, which we replace by their renormalized counterparts. The other divergent contribution could arise from the primitive divergences of the 1-particle reducible vertex function $\Gamma^{(2)}(k,t,0)$, defined by $G_{k}(t,0) \equiv \int G_{k}(t-t') \Gamma^{(2)}(k,t',0) \, dt'$. The superficial divergence of the diagrams contributing to $G_k(t,0)$ is $D = \nu_u(d-4) + \nu_g(d-6) - 2$ (where $\nu_u$ ($V_g$) is the number of $u$ ($g$) vertices respectively). This is always negative for $d \leq 6$. This implies that $G^B_k(t,0)$ does not get renormalized and $Z_0 = 1$. Consequently $\lambda$ stays at its mean-field value of $d$ for this conserved Heisenberg dynamics both with and without the torque $T$. We have shown that the inclusion of a torque to the ordering dynamics of a conserved Heisenberg magnet, is relevant both for quenches to $T = 0$ and $T > T_c$. The new zero temperature fixed point is characterised by exponents $z = 2$ and $\lambda \approx 5.15$. We have provided scaling arguments to understand these exponents and the crossover. We have shown that the class of approximate theories based on the Gaussian closure scheme which had been constructed to understand this zero temperature conserved dynamics, are inconsistent even when the torque is absent. On the other hand, the new critical fixed point is characterised by exponents $z = 4 - \varepsilon/2$ and $\lambda = d$ (where $\varepsilon = 6 - d$). Indeed $\lambda$ is always equal to $d$ for quenches to the critical point whenever the order parameter is conserved.

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