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Special Solution of the Mode-Coupling Equations for a Two-Component Magnetic System

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The validity of the vertex approximation for the nonlinear Langevin equations has been investigated in the special case of a two-component magnetic system without spatial correlation. The exact solution of the equation resulting from the vertex approximation is compared with that of the original equation. Agreement is found in the regime of small nonlinearity. In the opposite regime, especially near a critical slowing down, both solutions differ significantly.

KEY WORDS: Critical dynamics; Langevin equation; Kondo system.

The macroscopic behavior of magnetization densities, as, e.g., the conduction electron and impurity magnetization in a Kondo-like system, is governed by coupled Bloch equations,[1] which usually originate as a hydrodynamic limit from the microscopic equations of motion.[2] The neglect of quickly varying contributions in those derivations may be crucial under circumstances where the macroscopic coupling becomes prominent or, more serious, diverges because of weak approximations. It may be accounted for in a simplifying view by adding phenomenologically Gaussian random forces. Such a situation arises in Kondo theories applying a specific perturbation scheme which results in a coupling which is strong compared with slow relaxation rates for low temperatures.[3] Furthermore the random forces are a natural consequence of the fluctuation-dissipation theorem representing the origin of the dissipation terms in the Bloch equatios.

Recently Ginzburg–Landau equations of a similar type have become attractive in the context of dynamics of phase transitions. It opens a wide spectrum of methods to treat such nonlinear Langevin equations. One of

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them, the lowest-order vertex approximation of Kawasaki,[4] will be used here. The respective nonlinear integral equations for the correlation functions are generally nontrivial. They are solved for the special case where the volume of a homogenous independently fluctuating magnetization is characterized in size by a diffusion length to account for the diffusion of the mobile component. Equal lattice relaxation rates are assumed. The symmetric behavior of both components with respect to the lattice implies a linear dissipation of the total magnetization. Together with the detailed balance condition for the cross relaxation rates this yields a convolution integral solved by Laplace transformation. This solution could be used as a test for the validity of the vertex approximation.

In Section 1 the Bloch equations are introduced and supplemented by random forces. The mode-coupling equations of Kawasaki are derived in Section 2. The solution is presented in Section 3 and compared in Section 4 with the corresponding solution of the exact Bloch equations.

1. BLOCH EQUATIONS

The set of equations describing the system of coupled magnetization densities $\mathbf{S}_1, \mathbf{S}_2$ in zero field

$$\frac{d\mathbf{S}_1}{dt} = \alpha T \chi_1 \left(\mathbf{S}_2 \times \frac{\delta H}{\delta \mathbf{S}_1} \right) - \sum_k L_{1k} \frac{\delta H}{\delta \mathbf{S}_k} + \zeta_1$$

$$\frac{d\mathbf{S}_2}{dt} = \alpha T \chi_2 \left(\mathbf{S}_1 \times \frac{\delta H}{\delta \mathbf{S}_2} \right) - \sum_k L_{2k} \frac{\delta H}{\delta \mathbf{S}_k} + \zeta_2$$

uses the equilibrium Hamiltonian at temperature T

$$H = \frac{1}{2T} \int d^3x \left(\frac{1}{\chi_1} \mathbf{S}_1^2 + \frac{1}{\chi_2} \mathbf{S}_2^2 \right)$$

with susceptibilities χ_i, to yield the torque term representing the coupling with coefficient α and the dissipation term with matrix

$$L_{ik} = T \begin{bmatrix} \chi_1 \left(-D \nabla^2 + \frac{1}{T_{12}} + \frac{1}{T_{10}} \right) & -\chi_1 \frac{1}{T_{12}} \\ -\chi_2 \frac{1}{T_{21}} & \chi_2 \left(\frac{1}{T_{21}} + \frac{1}{T_{20}} \right) \end{bmatrix}$$

Only component $\mathbf{S}_1$ is assumed to show appreciable diffusion leading to the term with coefficient D. The cross relaxation rates satisfy the Onsager symmetry relation

$$\frac{\chi_2}{T_{21}} = \frac{\chi_1}{T_{12}}$$

Vanishing lattice relaxation rates $1/T_{10}$ and vanishing diffusion would imply local angular momentum conservation, $\mathbf{S}_1 + \mathbf{S}_2$, in the deterministic case. The Gaussian forces ζ_i

$$\langle \zeta_{i\mu}(t)\rangle = 0, \qquad \langle \zeta_{i\mu}(t)\zeta_{k\nu}(t')\rangle = 2L_{ik}\delta_{\mu\nu}\delta(t-t')$$

are correlated by the fluctuation-dissipation theorem, where the differential operator in the Onsager coefficients has to be suitably read in Fourier space.

With respect to the Kondo system, $\mathbf{S}_1$ represents the conduction electron and $\mathbf{S}_2$ the impurity magnetization. The coefficients α, D, and $1/T_{12}$ show logarithmic singularities in low-order perturbation theory for temperature approaching zero. Removing this divergency by diagram summation still leaves a strong effect of Kondo interaction around the Kondo temperature and below. The impurity susceptibility χ_2 increases according to a Curie law so that the fluctuations do not die out with decreasing temperature except at very low temperatures where the susceptibility saturates. The impurity relaxation $(1/T_{21})$ becomes slow for low temperatures. The lattice relaxation rates $1/T_{10}, 1/T_{20}$ are small and do not depend on temperature.[3]

2. MODE-COUPLING APPROXIMATION

A Lagrangian formalism[5] is applied to derive the mode-coupling equations governing the correlation functions

$$G_{q\alpha,q'\alpha'}(t-t') = \langle S_{q\alpha}(t)S_{q'\alpha'}(t')\rangle \tag{1}$$

for the Fourier quantities $S_{q\alpha}(t)$ of the densities. The letter $\alpha = (i, \mu)$ denotes the ith magnetization component with Cartesian index μ. The average in (1) with respect to the fluctuating forces can be replaced by a functional integration over a probability distribution of the magnetizations

$$W(\{S(t)\}, t_0 < t \leqslant t_1)\, d\{S\} \sim \int d\{i\tilde{S}\} \exp\left(-\int_{t_0}^{t_1} dt\, L\right) d\{S\} \tag{2}$$

determined by the Lagrangian

$$L = \int d^3x \left\{ -\sum_{\alpha\alpha'} \tilde{S}_\alpha(x,t) L_{\alpha\alpha'} \tilde{S}_{\alpha'}(x,t) + \sum_\alpha \tilde{S}_\alpha(x,t)\left[\dot{S}_\alpha(x,t) - V_\alpha\right] + \frac{1}{2}\sum_\alpha \frac{\partial V_\alpha}{\partial S_\alpha}(x,t)\right\} \tag{3}$$

with

$$V_{i\mu} = \sum_k \left(\alpha T \chi_i \sum_{\nu\eta} \epsilon_{\mu\nu\eta} S_{k\nu} \frac{\delta H}{\delta S_{i\eta}} - L_{ik}\frac{\delta H}{\delta S_{k\mu}}\right)$$
$$L_{\alpha\alpha'} \equiv L_{ii'}\delta_{\mu\mu'} \tag{4}$$

Extending the limits of integration in (2) $t_0 \to -\infty$, $t_1 \to +\infty$ the definition (1) coincides with the static equilibrium correlation function which will be the required quantity. The last term in (3) which reflects the Jacobian of the probabilities transformation does not depend on S_α and is omitted in the following. To obtain the correlation functions by differentiation of a common generating functional, response fields $\tilde{B}_\alpha(t)$ associated with the subsidiary magnetizations $\tilde{S}_\alpha(x,t)$ are introduced in addition to the physical fields $B_\alpha(t)$ by merely adding to L (3)

$$-\int d^3x \sum_\alpha \left[B_\alpha(t) S_\alpha(x,t) + \tilde{B}_\alpha(t) \tilde{S}_\alpha(x,t) \right] \tag{5}$$

Differentiating the generating functional, i.e., the logarithm of the $d\{S\}$ integral of $W(\{S\})$, with respect to B or $\tilde{B}$ yields the cumulants. Only connected diagrams have to be considered in the subsequent expansion in powers of the nonlinear contributions to V_α. The latter corresponds to the first term on the right-hand side of (4). It has a vanishing average with the unperturbed Lagrangian because of the antisymmetric unit tensor $\epsilon_{\mu\nu\eta}$ which excludes self-loops. The zero-order propagators derive from the unperturbed, Gaussian probability

$$\begin{aligned} \langle S_{q\alpha}(t) \tilde{S}_{q'\alpha'}(t') \rangle_0 &= (2\pi)^3 \delta(q+q') \delta_{\mu\mu'} \Theta(t-t') \left(e^{-\gamma(t-t')}\right)_{ii'} \\ &= \tilde{G}^0_{q\alpha,q'\alpha'}(t-t') = \alpha t \overset{q}{\longleftarrow\!\sim} \alpha' t' \end{aligned} \tag{6}$$

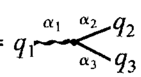
$$\begin{aligned} \langle S_{q\alpha}(t) S_{q'\alpha'}(t') \rangle_0 &= T\left(\tilde{G}^0_{q\alpha,q'\alpha'}(t-t') \chi_{i'} + \tilde{G}^0_{q'\alpha',q\alpha}(t'-t) \chi_i \right) \\ &= G^0_{q\alpha,q'\alpha'}(t-t') = \alpha t \overset{q}{\longleftarrow} \alpha' t' \end{aligned} \tag{7}$$

$$\gamma_{ik} \equiv \frac{1}{T\chi_k} L_{ik}, \qquad S_\alpha(x,t) = \int_q S_{q\alpha}(t) e^{iqx}, \qquad \int_q \equiv \int \frac{d^3q}{(2\pi)^3}, \qquad \alpha = (i, \mu)$$

The perturbation expansion for the correlation function (1) involves the pair contractions of powers of the bare interaction vertex

$$\int_{-\infty}^{+\infty} dt\, L_1 = \sum_{\alpha_1 \ldots \alpha_3} \int_{-\infty}^{+\infty} dt \int_{q_1} \cdots$$

$$\times \int_{q_3} (2\pi)^3 \delta(q_1 + q_2 + q_3) C_{\alpha_1\alpha_2\alpha_3} \tilde{S}_{q_1\alpha_1}(t) S_{q_2\alpha_2}(t) S_{q_3\alpha_3}(t)$$

$=$  (8)

$$C_{\alpha_1\alpha_2\alpha_3} \equiv \tfrac{1}{2} \alpha \epsilon_{\mu_1\mu_2\mu_3} \left(\delta_{i_1 i_2} - \delta_{i_1 i_3} \right) \tag{9}$$

and of the two external legs with suitable numerical factors.[6] The integral equations of the mode-coupling theory may be obtained by partial summation of diagrams, especially neglecting all vertex corrections to the self-energy Σ:

$\Sigma =$ 

Thus in shorthand notation

$$\tilde{G} = \tilde{G}^0 + \tilde{G}^0 \Sigma \tilde{G}$$
$$G = G^0 + \tilde{G}^0 \Sigma G \tag{10}$$

especially for the first equation

$$\tilde{G}_{\alpha\alpha'}(q,t) = \Theta(t)\delta_{\mu\mu'}(e^{-\gamma t})_{ii'} + 4 \sum_{\alpha_1 \ldots \alpha_3'} C_{\alpha_1\alpha_2\alpha_3} C_{\alpha_1'\alpha_2'\alpha_3'}$$
$$\times \int_0^t dt_1 \int_0^{t_1} dt_1' \int_{q_1} \tilde{G}^0_{\alpha\alpha_1}(q, t - t_1) G_{\alpha_2\alpha_2'}(q_1, t_1 - t_1')$$
$$\times \tilde{G}_{\alpha_3\alpha_1'}(q - q_1, t_1 - t_1') \tilde{G}_{\alpha_3'\alpha'}(q, t_1') \tag{11}$$

omitting the factor $(2\pi)^3\delta(q + q')$ in the definition of $G(q,t)$. The requirement of causality can be fulfilled by the solution to (10). It connects both correlation functions by

$$\tilde{G}_{\alpha\alpha'}(q,t) T \chi_{i'} = \Theta(t) G_{\alpha\alpha'}(q,t) \tag{12}$$

so that $G, \tilde{G}$ decouple and only $\tilde{G}$ arises in (11). It represents a nonlinear integral equation for the time-dependent matrix $\tilde{G}$.

3. SOLUTION

As an ansatz the correlation function is taken to be diagonal with respect to the vector components of the magnetizations, i.e.,

$$\tilde{G}_{\alpha\alpha'}(q,t) = \delta_{\mu\mu'} g_{ii'}(t)\Theta(t), \qquad g_{ii'}(0) = \delta_{ii'} \tag{13}$$

and thus (11) leads to

$$\left(\frac{d}{dt} + \gamma\right) g(t) = 2\alpha^2 T \int_0^t dt_1 \int_{q_1} \left[g(t - t_1)\chi - \mathrm{Tr}\left(g(t - t_1)\chi\right) \right] g(t - t_1) g(t_1) \tag{14}$$

with matrix χ defined by $\chi_{ik} \equiv \chi_i$. In the following the diffusion term in γ is neglected. In addition the lattice relaxation rates are assumed to be equal ($T_{10} = T_{20}$). From that the linear dissipation of the total magnetization follows

$$\left(\frac{d}{dt} + \frac{1}{T_{10}}\right)(g_{1k} + g_{2k}) = 0 \tag{15}$$

Furthermore one derives from (14) an expression reflecting the detailed balance for this symmetric system

$$\chi_1 g_{21} = \chi_2 g_{12} \tag{16}$$

Only one quantity

$$g_- = g_{11} - g_{12} \tag{17}$$

remains to be calculated. From (14) using (15), (16), (17) the integral equation

$$\left[\frac{d}{dt} + \frac{1}{T_{10}} + \frac{1}{T_{12}}\left(1 + \frac{\chi_1}{\chi_2}\right)\right] g_-$$
$$= -2\tilde{\alpha}^2 T(\chi_1 + \chi_2)\int_0^t dt'\, e^{-(t-t')/T_{10}} g_-(t - t') g_-(t') \tag{18}$$

with $g_-(0) = 1$ follows. The integrand in (14) is assumed to be independent of momentum below a cutoff which corresponds to an inverse spin diffusion length $(DT_{10})^{-1/2}$. Thus the q-integral is incorporated in a modified coupling constant $\tilde{\alpha}^2 \equiv \alpha^2 (DT_{10})^{-3/2}$. Equation (18) can be solved by Laplace transformation

$$-1 + \left[s + \frac{1}{T_{10}} + \frac{1}{T_{12}}\left(1 + \frac{\chi_1}{\chi_2}\right)\right]\hat{g}_-(s)$$
$$= -2\tilde{\alpha}^2 T(\chi_1 + \chi_2)\,\hat{g}_-\left(s + \frac{1}{T_{10}}\right)\hat{g}_-(s) \tag{19}$$

This difference equation with respect to the increment $1/T_{10}$ of s is simplified introducing the quantities

$$\nu = \left[s + \frac{1}{T_{12}}\left(1 + \frac{\chi_1}{\chi_2}\right)\right] T_{10}, \qquad f_\nu = 2\tilde{\alpha}^2 T(\chi_1 + \chi_2) T_{10}\hat{g}_-(s)$$
$$x = 2T_{10}\left[2\tilde{\alpha}^2 T(\chi_1 + \chi_2)\right]^{1/2} \tag{20}$$

and yields

$$f_{\nu+1} + (\nu + 1) = x^2/4f_\nu \tag{21}$$

which is reduced with a simple trick borrowed from the theory of continued fractions. The unknown function is replaced by a fraction

$$f_\nu = \frac{u_\nu}{v_\nu} \tag{22}$$

and comparing nominator and denominator of the resulting equation, a solution is obtained by solving the linear difference equations

$$v_{\nu-1} - v_{\nu+1} = \frac{2\nu}{x} v_\nu$$
$$u_\nu = \frac{x}{2} v_{\nu+1} \tag{23}$$

The first equation of (23) is identical with the recurrence formula for the Bessel function with imaginary argument, $I_\nu(x)$. Thus one solution of (19) reads

$$\hat{g}_-(s) = \frac{2T_{10}}{x} I_{\nu+1}(x)/I_\nu(x) \tag{24}$$

According to (20) the complex variable s of the Laplace transform arises in the order of the Bessel function while the argument x is a positive parameter as long as the coupling does not vanish. The solution (24) shows for large $|s|$ the asymptotic behavior as implied by (19), $\hat{g}(s) \propto 1/s$. The continued fraction following from (21) converges as $\nu \to +\infty$ and thus defines uniquely the solution f_ν for $\nu > -1$ on the real axis. Therefore (24) represents the unique solution for s complex being analytic with the exception of the zeros of the Bessel function.

The case of zero coupling, $x = 0$, is trivial and (24) leads to a linear relaxation $g_-(t)$ coinciding with the rate on the left-hand side of (18). The large t behavior follows from that pole of (24) which has the largest real part with respect to s. Up to order $\tilde{\alpha}^2$ the decay rate of $g_-(t)$ is given by

$$-s_0 = \frac{1}{T_{10}} + \frac{1}{T_{\text{cr}}} + \omega_\alpha^2 T_{10}, \qquad \tilde{\alpha} \to 0 \tag{25}$$

with $\omega_\alpha^2 \equiv 2\tilde{\alpha}^2 T(\chi_1 + \chi_2)$ being the average of the squared (coupling induced) precession frequency and $T_{\text{cr}}^{-1} \equiv T_{12}^{-1}(1 + \chi_1/\chi_2)$ an effective cross relaxation rate. A further quantity measuring an average decay time can be extracted immediately from the Laplace transform

$$\tau_0 \equiv \int_0^\infty g_-(t)\, dt = \hat{g}_-(0) \tag{26}$$

which yields in order $\tilde{\alpha}^2$ a slightly different expression

$$\frac{1}{\tau_0} = \frac{1}{T_{10}} + \frac{1}{T_{\text{cr}}} + \frac{\omega_\alpha^2 T_{10} T_{\text{cr}}}{2T_{\text{cr}} + T_{10}}, \qquad \tilde{\alpha} \to 0 \tag{27}$$

Strong coupling leads asymptotically to

$$\frac{1}{\tau_0} = \omega_\alpha + \frac{1}{4}\left(\frac{1}{T_{10}} + \frac{2}{T_{\text{cr}}}\right), \qquad \tilde{\alpha} \to \infty \tag{28}$$

The Laplace transform is easily inverted for the first few terms of an expansion with respect to a small lattice relaxation rate $1/T_{10}$

$$g_-(t) = \frac{1}{\omega_\alpha t} e^{-t/T_{cr}} \left[J_1(2\omega_\alpha t) - \frac{1}{2T_{10}} \sin(2\omega_\alpha t) \right] \tag{29}$$

showing an oscillatory behavior and a slowing down to a $t^{-3/2}$ power law for vanishing relaxation rates T_{10}^{-1}, T_{cr}^{-1}. The latter is quite different from the deterministic result of an undamped precession of the individual magnetizations with respect to the total magnetization.

4. CONCLUSION

To get a feeling for the validity of the vertex approximation it seems to be useful to compare its results with calculations which are performed on the original Bloch equations in special solvable cases. Under the restriction leading to (29) it is possible to obtain also an exact solution of the equations cited in Section 1. In the Fourier representation along the same reasoning only the small momentum components are considered and taken to be independent of momentum. Below the cutoff the momentum index drops out and α has to be replaced by $\tilde{\alpha}$. Introducing

$$\mathbf{S} \equiv \mathbf{S}_1 + \mathbf{S}_2, \qquad \mathbf{s} \equiv \mathbf{S}_1/T_{12} - \mathbf{S}_2/T_{21}$$

$$\boldsymbol{\eta} \equiv \boldsymbol{\zeta}_1 + \boldsymbol{\zeta}_2, \qquad \boldsymbol{\zeta} \equiv \boldsymbol{\zeta}_1/T_{12} - \boldsymbol{\zeta}_2/T_{21}$$

The component of the total magnetization yields

$$\mathbf{S} = \int_0^t dt_1 \exp[-(t - t_1)/T_{10}] \boldsymbol{\eta}(t_1) \equiv \mathbf{e}(t)$$

if the initial value is set equal to zero. It only consists of a weakly fluctuating part as can be seen from the correlation functions given in Section 1.

$$\langle e_\mu(t) e_\nu(t') \rangle = \delta_{\mu\nu} T(\chi_1 + \chi_2) \{ \exp(-|t - t'|/T_{10}) - \exp[-(t + t')/T_{10}] \}$$

Performing the limit $t, t' \to \infty$ with finite $(t - t')$ to get rid of the initial values, the correlation time increases with increasing T_{10}. In the limit $T_{10} \to \infty$ the correlation function becomes constant in time yielding time-independent, Gaussian distributed random variables e_μ. As a consequence the magnetization difference $\mathbf{s}$ obeys a linear differential equation with constant random coefficients following from the Bloch equations

$$\dot{\mathbf{s}} = \tilde{\alpha} \mathbf{s} \times \mathbf{e} - \mathbf{s}/T_{cr} + \boldsymbol{\zeta}$$

where

$$\langle \zeta_\mu(t) \zeta_\nu(t') \rangle = \frac{2T\chi_1}{T_{12} T_{cr}^2} \delta_{\mu\nu} \delta(t - t')$$

It is straightforward to integrate this differential equation yielding the correlation function

$$\langle s_\mu(t)s_\nu(t')\rangle = \delta_{\mu\nu}\frac{T\chi_1}{3T_{12}T_{cr}}\exp(-|t-t'|/T_{cr})\Big(1+2\Big\langle\cos\tilde{\alpha}\sqrt{\mathbf{e}^2}\,(t-t')\Big\rangle\Big) \tag{30}$$

with

$$\Big\langle\cos\tilde{\alpha}\sqrt{\mathbf{e}^2}\,(t-t')\Big\rangle = \Big[1-\tfrac{1}{2}\omega_\alpha^2(t-t')^2\Big]\exp\Big[-\tfrac{1}{4}\omega_\alpha^2(t-t')^2\Big]$$

Because of definition the following relation holds:

$$\langle s_\mu(t)s_\nu(t')\rangle = \delta_{\mu\nu}\frac{T\chi_1}{T_{12}T_{cr}}\,g_-(t-t'), \qquad t \geqslant t'$$

and the result in (29) for $1/T_{10}=0$ can be compared with (30). The solution of the vertex approximation differs qualitatively from the solution of the Bloch equations and shows a remarkably slower decay than the latter in the short time behavior. As is to be expected, both expressions coincide within quadratic order of the coupling constant. The difference increases with increasing coupling strength. With respect to the long time behavior the vertex approximation works in the regime $T_{cr}\omega_\alpha \ll 1$, i.e., as long as the precession period is much greater than the relaxation time. In the opposite regime, especially in the case of a critical slowing down of the relaxation rate, this approximation fails. There seems to be little reason that this situation improves if the diffusion with its momentum dependence is properly taken into account.

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