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Nonlinear Responses in Magnetic Systems

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The present paper reviews some general characteristic properties of nonlinear responses and discusses some interesting aspects of those in magnetic systems such as spin glasses, random spin systems, Heisenberg magnets and kinetic Ising systems. In particular, nonlinear responses of quantum systems are expressed in terms of higher-order quantum derivatives. The magnetization of the Heisenberg model in the presence of a magnetic field is shown to be expressed in terms of the transverse magnetic fluctuation in the presence of a magnetic field.

KEYWORDS: nonlinear response, magnetic system, quantum analysis, Heisenberg model, spin-glass

§1. General Expressions of Nonlinear Responses

It will be instructive to review general expressions of equilibrium and nonequilibrium nonlinear responses.

i) Nonlinear responses in equilibrium systems

The average $\langle Q\rangle$ in an equilibrium system for a physical quantity Q is given by

$$\langle Q\rangle = \mathrm{Tr}\, Q\rho, \tag{1.1}$$

where the equilibrium density matrix $\rho = \exp[-\beta(\mathcal{H} - HQ)]$ with $\beta = 1/k_{\mathrm{B}}T$ is expanded with respect to an external field H conjugate to Q in the form[1)]

$$\rho = \sum_{n=0}^{\infty} \frac{(-H)^n}{n!} \frac{d^n e^{-\beta\mathcal{H}}}{d\mathcal{H}^n} : \underbrace{Q\cdots Q}_{n}, \tag{1.2}$$

where the quantum derivative $d^n e^{-\beta\mathcal{H}}/d^n\mathcal{H}$ is defined[2–6)] using the following higher-order quantum derivative $d^n f(A)/d^n A$:

$$\frac{d^n f(A)}{dA^n} = n! \int_0^1 dt_1 \int_0^{t_1} dt_2 \cdots \cdots \int_0^{t_{n-1}} dt_n f^{(n)}(A - t_1\delta_1 - \cdots - t_n\delta_n), \tag{1.3}$$

where $f^{(n)}(x)$ denotes the n-th derivative of $f(x)$ and the inner derivation δ_j is defined by

$$\delta_j : dA\cdot dA \cdots\cdots dA = dA\cdot dA\cdots\cdots(\delta_A dA)\cdots\cdots dA. \tag{1.4}$$

Here, δ_A is defined by $\delta_A Q = [A,Q] = AQ - QA$. Using the quantum derivative (1.3), we have the following operator Taylor expansion formula:[1–6)]

$$f(A + xB) = \sum_{n=0}^{\infty} \frac{x^n}{n!} \frac{d^n f(A)}{dA^n} : B^n, \tag{1.5}$$

These formulas will be used efficiently in discussing nonlinear responses of magnetic systems.

ii) Nonlinear responses in nonequilibrium systems

The nonlinear response $\langle Q\rangle_t$ in a nonequilibrium system described by the time-dependent Hamiltonian

$$\mathcal{H}(t) = \mathcal{H} - A\,F(t), \tag{1.6}$$

is obtained through the density matrix $\rho(t)$ satisfing the von Neumann equation

$$i\hbar \frac{\partial}{\partial t} \rho(t) = [\mathcal{H}(t), \rho(t)]. \tag{1.7}$$

In order to study the time-dependent nonlinear response for (1.6), it is convenient to introduce the so-called "entropy operator" $\eta(t)$ as $\rho(t) = \exp(-\eta(t))$. Then, $\eta(t)$ is shown[1)] to satisfy the same equation as (1.7), using the quantum analysis. This fact gives the following perturbational expansion of $\eta(t)$, namely the exponential perturbation scheme:[1)]

$$\eta(t) = \Phi + \beta\mathcal{H} + \eta_1(t) + \eta_2(t) + \cdots + \eta_n(t) + \cdots \tag{1.8}$$

with a normalization constant Φ and

$$\eta_n(t) = -\frac{\beta}{(i\hbar)^{n-1}} \int_{-\infty}^{0} e^{\varepsilon s} ds F(t+s) \int_0^s dt_1 \int_0^{t_1} dt_2 \cdots \cdots \int_0^{t_{n-2}} dt_{n-1} F(t+t_1)\cdots F(t+t_{n-1}) \times \delta_{A(t_1)}\delta_{A(t_2)}\cdots\delta_{A(t_{n-1})}\dot{A}(s), \tag{1.9}$$

with the hyperoperator $\delta_{A(t)}$ and with $\dot{A} = (i\hbar)^{-1}\delta_A\mathcal{H}$.

As was pointed out in Ref.1, the first-order term $\eta_1(t)$ gives Zubarev's theory in the above situation. The scheme (1.8) is a renormalized expansion, because even the "first-order" density matrix $\rho_1(t) \equiv \exp(-\Phi - \beta\mathcal{H} - \eta_1(t))$ in the above sense contains partially terms up to infinite order with respect to the external field H.

§2. Nonlinear Responses to Local Fields and Random Local Fields in the Ising Model

In the present section, we explain nonlinear responses of local fields in the Ising model as a preliminary example of more general formulations in quantum systems.

The simplest example is an expression of the local magnetization at the site k, $m_k = g\mu_B\langle S_k\rangle$ as a function of a local field H_j. It is easily shown that the average $\langle S_k\rangle$ in the presence of H_j is given by

$$\langle S_k\rangle = \frac{\langle S_k\rangle_0 + \langle S_k S_j\rangle_0 \tanh h_j}{1 + \langle S_j\rangle_0 \tanh h_j}, \tag{2.1}$$

where $h_j = \beta\mu_B H_j$ and $\langle Q\rangle_0$ and $\langle Q\rangle$ denote the canonical averages for the Hamiltonians $\mathcal{H}_0$ and $\mathcal{H}(= \mathcal{H}_0 - \mu_B H_j S_j)$. Equation (2.1) holds even when $\mathcal{H}_0$ contains magnetic fields at any lattice points. If $k = j$, we have

$$\langle S_j\rangle = \frac{\langle S_j\rangle_0 + \tanh h_j}{1 + \langle S_j\rangle_0 \tanh h_j}. \tag{2.2}$$

These expressions hold in the whole range of the local field H_j. We can derive many other expressions for canonical averages of any spin operators, $\langle S_{j_1}\cdots S_{j_n}\rangle$.

These results will be extended later to quantum spin systems.

When H_j is a random local field, we have

$$\langle\langle S_k\rangle\rangle_{H_j} = \left\langle \frac{\langle S_k\rangle_0 + \langle S_k S_j\rangle_0 \tanh(\beta\mu_B H_j)}{1 + \langle S_j\rangle_0 \tanh(\beta\mu_B H_j)} \right\rangle_{H_j}. \tag{2.3}$$

If $\mathcal{H}$ does not contain any magnetic field, then we have $\langle S_j\rangle_0 = \langle S_k\rangle_0 = 0$. Thus, we arrive at the results

$$\langle\langle S_k\rangle\rangle_{H_j} = \langle S_k S_j\rangle_0 \langle \tanh(\beta\mu_B H_j)\rangle_{H_j}, \tag{2.4}$$

and

$$\langle\langle S_k\rangle^2\rangle_{H_j} = \langle S_k S_j\rangle_0^2 \langle \tanh^2(\beta\mu_B H_j)\rangle_{H_j}, \tag{2.5}$$

or

$$\langle\langle S_k\rangle^2\rangle_J = \langle\langle S_k S_j\rangle_0^2\rangle_J \tanh^2(\beta\mu_B H_j) \tag{2.6}$$

for a fixed value of H_j. Here $\langle\cdots\rangle_J$ denotes the random average over the distribution of exchange interactions $\{J_{ij}\}$.

These results will be instructive in discussing the nonlinear response in spin glasses.

§3. Nonlinear Responses in Quantum Spin Systems

We can show, even in quantum spin systems, that there are some cases in which nonlinear responses can be exactly expressed in terms of a finite number of spin correlations.

i) Nonlinear responses in spin systems with local constants of motion.

We consider the following Hamiltonian

$$\mathcal{H} = -\sum_{\langle jk\rangle} J_{jk} S_j^z S_k^z - g\mu_B \sum_j H_j S_j^z - \Gamma_i S_i^x \equiv \mathcal{H}_u - \Gamma_i S_j^x \tag{3.1}$$

for some fixed site i. Here $\langle jk\rangle$ denotes the nearest neighbour interactions. Clearly there exists a local constant of motion, $\mathcal{H}_{\rm loc}$ defined by

$$\mathcal{H}_{\rm loc} = -\sum_k^{\rm all} J_{jk} S_i^z S_k^z - g\mu_B H_i S_i^z - \Gamma_i S_i^x \equiv \mathcal{H}_i - \Gamma_i S_i^x \tag{3.2}$$

for any value of spin. The remaining Hamiltonian $\mathcal{H}_{\rm r}$ is given by $\mathcal{H}_{\rm r} = \mathcal{H} - \mathcal{H}_{\rm loc}$ and it is different from the uniform Ising Hamiltonian $\mathcal{H}_{\rm u}$ by $\mathcal{H}_i$, namely $\mathcal{H}_{\rm r} = \mathcal{H}_{\rm u} - \mathcal{H}_i$. Note that $[\mathcal{H}_{\rm u}, \mathcal{H}_i] = 0$, because they are both of Ising type. Thus, we have

$$\begin{aligned}\langle Q\rangle &= {\rm Tr}\, Q\, e^{-\beta\mathcal{H}}/{\rm Tr}\, e^{-\beta\mathcal{H}} \\ &= \langle Q\, e^{-\beta\mathcal{H}_{\rm loc}} e^{\beta\mathcal{H}_i}\rangle_{\rm u} / \langle e^{-\beta\mathcal{H}_{\rm loc}} e^{\beta\mathcal{H}_i}\rangle_{\rm u}\end{aligned} \tag{3.3}$$

for any spin operator Q. The average $\langle Q\rangle_u$ denotes the canonical average for the Hamiltonian $\mathcal{H}_u$. It is easy to confirm that both of the numerator and denominator of (3.3) are expressed in terms of a finite number of spin correlation functions.

There are many other such examples, say an alternating transverse Ising model,

$$\mathcal{H} = -\sum_{\langle jk\rangle} J_{jk} S_j^z S_k^z - g\mu_B \sum_k H_k S_k^z - \sum_{j\in A} \Gamma_j S_j^x \tag{3.4}$$

for a bipartite lattice composed of A and B sublattices. There are an infinite number of local constants of motion in this Hamiltonian. Namely the following local Hamiltonian

$$\mathcal{H}_j = -\sum_{k\in B} J_{jk} S_j^z S_k^z - g\mu_B H_j S_j^z - \Gamma_j S_j^x \tag{3.5}$$

commutes with $\mathcal{H}$ for any j of the A sublattice.

More detailed calculations will be reported elsewhere. For some exact treatments of the uniform transverse Ising chain, see ref. 7 and references cited therein.

ii) Nonlinear response in the Heisenberg model

We consider here the following Heisenberg model

$$\mathcal{H} = -\sum J_{ij}\, \boldsymbol{S}_i \cdot \boldsymbol{S}_j - g\mu_B H \sum_{j=1}^N S_j^z \tag{3.6}$$

with arbitrary spins $\{S_j\}$. As is well known, the second Zeeman term in (3.6) commutes with the first term in (3.6). Using this symmetry and the identitiy[8]

$$\langle [A, B]\rangle = \int_0^\beta \langle {\rm e}^{\lambda\mathcal{H}} [\mathcal{H}, B]\, {\rm e}^{-\lambda\mathcal{H}} A\rangle d\lambda \tag{3.7}$$

obtained directly or from the quantum derivative of ${\rm e}^{-\beta\mathcal{H}}$ with respect to $\mathcal{H}$, we obtain

$$\langle S_j^z\rangle = \tanh(\beta\mu_B H) \sum_{i=1}^N \langle S_i^x S_j^x + S_i^y S_j^y\rangle \tag{3.8}$$

for $g = 2$ after straight-forward but lengthy calculations. Namely the local moment in the presence of a magnetic field is expressed in terms of the transverse correlation functions in the presence of a magnetic field. Thus, the total moment $S^z = \sum S_j^z$ is expressed in the form[9]

$$\langle S^z\rangle = \tanh(\beta\mu_B H)\langle (S^x)^2 + (S^y)^2\rangle. \tag{3.9}$$

This indicates that the nonlinear response is expressed by the quantum fluctuation in the presence of a magnetic field. This holds in the whole range of the magnetic field.

§4. Nonlinear Susceptibility in Spin Glasses

As is well known, the linear susceptibility $\chi_0(T)$ does not show any divergent singularity at the spin-glass transition point. It was pointed out by the present author[10] that the nonlinear susceptibility $\chi_2(T)$ defined in

$$m = \chi_0(T)H + \chi_2(T)H^3 + \cdots \tag{4.1}$$

for the magnetization m per site in a magnetic field H is related to the spin-glass response $\chi_{\rm sg}$ as

$$\chi_2(T) \propto -\chi_{\rm sg}(T). \tag{4.2}$$

Here, $\chi_{\rm sg}(T)$ is defined in the expansion

$$q \equiv \langle\langle S_j^z\rangle_H^2\rangle_J = \chi_{\rm sg}(T)H^2 + \cdots \tag{4.3}$$

for the spin-glass order parameter q above the critical point $T_{\rm sg}$. Here, $\langle\cdots\rangle_J$ denotes the average over the distribution of the random exchange interactions $\{J_{ij}\}$. As is seen from (2.6) or more rigorously from Appendix, the spin-glass susceptibility $\chi_{\rm sg}(T)$ is expressed in terms of the spin-glass correlation function as

$$\chi_{\rm sg}(T) = (\beta\mu_{\rm B})^2\sum_{j=1}^{N}\langle\langle S_i^z S_j^z\rangle_0^2\rangle_J \tag{4.4}$$

for $T \geq T_{\rm sg}$. This diverges[10–12] at the transition point $T_{\rm sg}$. Therefore, the nonlinear susceptibility $\chi_2(T)$ shows negative divergence.[10] This prediction was confirmed experimentally by Miyako et al.[13] Thus, the spin-glass phase transition is characterized by the negative divergence of the nonlinear susceptibility.

More explicitely, the spin-glass order parameter q is expressed as[14]

$$q = \frac{t}{2}\{(1+\frac{2h^2}{t^2})^{1/2} - 1\} \tag{4.5}$$

with $t = (T - T_{\rm sg})/T_{\rm sg}$ and $h = \chi_0(T_{\rm sg})H/\mu_{\rm B}$ for the SK model. The above scaling law explains well the divergence of $\chi_{\rm sg}(T)$ at $T_{\rm sg}$, and consequently the negative divergence of the nonlinear susceptibility is shown to appear through the relation (4.2).

§5. Nonlinear Relaxation in the Kinetic Ising Model

First we review the critical slowing down in the linear response for the kinetic Ising model. For example, the relaxation time τ of the magnetization m of the kinetic Ising model shows the following anomaly

$$\tau \sim \frac{1}{|T - T_{\rm c}|^{\Delta}} \tag{5.1}$$

near the critical point.

According to the van Hove theory, τ is proportional to the susceptibility $\chi_0(T)$ and consequently we have $\Delta = \gamma$ for the susceptibility exponent γ. However, in 1969 Yahata and the present author[15] found that Δ is different from γ, namely that there exists an intrinsic dynamical critical exponent, at least in the kinetic Ising model. Many papers[16] have been published to confirm this statement.

According to the renormalization group theory,[17] we have

$$\Delta - \gamma = \frac{1}{18}\varepsilon^2 \log(\frac{4}{3}) + \cdots \tag{5.2}$$

in d dimensions, for $\varepsilon = 4 - d$. This shows that $\Delta > \gamma$, at least near $d = 4\,(d < 4)$.

In order to study the linear and nonlinear relaxation in a unified way, the present author[18] defined the relaxation τ by

$$\tau = \int_0^\infty \frac{m(t) - m(\infty)}{m(0) - m(\infty)}\,dt\,, \tag{5.3}$$

for example, for the magnetization $m(t)$ as a function of time t. Then, the linear exponent $\tau^{(l)}$ and nonlinear exponent $\tau^{(nl)}$ satisfy the relation[19]

$$\Delta^{(l)} - \Delta^{(nl)} = \beta. \tag{5.4}$$

The present author[20] proposed the following "dynamic finite-size scaling":

$$m(t) = t^{-\psi}m\,(h\,\varepsilon^{\beta\delta}\,,\,\varepsilon^{\Delta}t\,,L^{-z}t) \tag{5.5}$$

for a magnetic field h and size L. Here, $\psi = \beta/\Delta = \beta/\nu z$. This dynamic finite-size scaling law has been found recently to be very useful[16] in evaluating even equilibrium critical exponents $\beta\,,\gamma$, ν and δ.

§6. Summary and Discussion

In the present paper, we have reviewed a general expression of nonlinear responses in terms of quantum derivatives and also nonlinear responses in nonequilibrium systems. Nonlinear responses to local fields and random local fields in the Ising model have been formulated. Nonlinear responses in quantum spin systems are also discussed using the symmetry property of the relevant system, namely the existence of a constant of motion. The negative divergence of the nonlinear susceptibility of spin glasses has been discussed from our viewpoint of nonlinear responses in magnetic systems.

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Appendix

The average $\langle S_k^z\rangle$ is expressed as

$$\langle S_k^z\rangle_H = \sum_{j=1}^{N}\langle S_k^z S_j^z\rangle_0\,\beta\mu_{\rm B}H \tag{A·1}$$

in the linear regime of a uniform external field H. Then we have

$$\begin{aligned}\langle\langle S_k^z\rangle_H^2\rangle_J &= (\beta\mu_{\rm B}H)^2\sum_{i,j}\langle\langle S_k^z S_i^z\rangle_0\langle S_k^z S_j^z\rangle_0\rangle_J \\ &= (\beta\mu_{\rm B}H)^2\sum_{i,j}\langle\langle S_k^z S_j^z\rangle_0\langle S_k^z S_j^z\rangle_0\rangle_J\,\delta_{ij} \\ &= (\beta\mu_{\rm B}H)^2\sum_{j=1}^{N}\langle\langle S_k^z S_j^z\rangle_0^2\rangle_J. \end{aligned} \tag{A·2}$$

Thus, we arrive at (4.4).

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