ON THE QUANTUM-STATISTICAL THEORY OF SPIN DIFFUSION

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Abstract

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L. L. BUIISHVILI, N. P. GIORGADZE

ON THE QUANTUM-STATISTICAL THEORY OF SPIN DIFFUSION

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In paper ([1]) the coefficient of spin diffusion was expressed in terms of moments of the corresponding correlation functions. In so doing, the reasoning was based on certain models requiring the introduction of auxiliary variable fields, and some assumptions were adopted which substantially restrict the generality of the conclusion. At the same time, considerable progress has recently been achieved in the development of the general theory of the statistical physics of irreversible processes ([2]).

In this connection it is of interest to obtain an expression for the diffusion coefficient starting from the general method of the nonequilibrium statistical operator proposed by D. N. Zubarev ([3]) and used for the investigation of diffusion of magnetic moment in paper ([4]).

Let H be the Hamiltonian of a certain spin system, and let this system be regarded as an aggregate of separate weakly interacting subsystems H^s, so that $H = \sum H^s$.

For example, in a strong magnetic field such subsystems are the Zeeman energy and the secular part of the dipole-dipole reservoir, or the Zeeman energy and the exchange reservoir if there is a strong exchange interaction. In a weak magnetic field the Zeeman energy and the dipole-dipole reservoir should be regarded as a single subsystem. It should be noted here that diffusion within each subsystem is due to the secular part of the dipole-dipole interaction or to the exchange interaction.

Let us introduce the Hamiltonian density of subsystem s

$$H^s(\mathbf{x}) = \sum_i \delta(\mathbf{x} - \mathbf{x}_i) H_i^s, \tag{1}$$

defined so that

$$\int d\mathbf{x}\, H^s(\mathbf{x}) = H^s.$$

Here, in the case of the Zeeman subsystem, H_i^s is the Zeeman energy of site i, while in the case of the dipole-dipole reservoir it is one half of the energy associated with site i.

Following now paper ([3]), in the high-temperature approximation for the statistical operator we obtain:

$$\rho = (1/\operatorname{Sp} 1)\left\{1 - \sum_{s'} \int d\mathbf{x}'\, \beta^{s'}(\mathbf{x}')H^{s'}(\mathbf{x}') + \right.$$
$$\left. + \sum_{s'} \int d\mathbf{x}' \int_{-\infty}^{0} dt'\, e^{\varepsilon t'} \beta^{s'}(\mathbf{x}')K^{s'}(\mathbf{x}'t')\right\} \quad (\varepsilon > 0), \tag{2}$$

where

$$K^s(\mathbf{x}) = \frac{1}{i}\,[H^s(\mathbf{x})H],$$

and $\beta^s(\mathbf{x})$ is the inverse temperature of subsystem s.

The temporal evolution of the temperature of subsystem s is determined by the equation

$$\frac{\partial \overline{H^s(\mathbf{x})}}{\partial t} = \overline{K^s(\mathbf{x})} \tag{3}$$

together with the assumption of quasistaticity of the process, where

$$\overline{K^s(\mathbf{x})} = \operatorname{Sp} \rho K^s(\mathbf{x}) = \sum_{s'} \int d\mathbf{x}' \int_{-\infty}^{0} dt'\, e^{\varepsilon t'} \left\langle K^s(\mathbf{x})K^{s'}(\mathbf{x}'t')\right\rangle \beta^{s'}(\mathbf{x}'),$$

$$\overline{H^s(\mathbf{x})} = \operatorname{Sp} \rho H^s(\mathbf{x}) = -\sum_{s'} \int d\mathbf{x}' \left\langle H^s(\mathbf{x})H^{s'}(\mathbf{x}')\right\rangle \beta^{s'}(\mathbf{x}'), \tag{4}$$

$$\langle A\rangle = \operatorname{Sp} A/\operatorname{Sp} 1.$$

Substituting (2) into (4), we obtain

$$\overline{K^s(\mathbf{x})} = \sum_{ij} \sum_{s'} \delta(\mathbf{x} - \mathbf{x}_i) \int_{-\infty}^{0} dt\, e^{\varepsilon t} \left\langle K_i^s K_j^{s'}(t)\right\rangle \beta^{s'}(\mathbf{x}_j),$$

$$\overline{H^s(\mathbf{x})} = -\sum_{ij}\sum_{s'} \delta(\mathbf{x}-\mathbf{x}_i) \left\langle H_i^s H_j^{s'} \right\rangle \beta^{s'}(\mathbf{x}_j), \tag{5}$$

where $K_i^s = \dfrac{1}{i}[H_i^{sH}]$.

By virtue of the spatial homogeneity of the system under consideration, $\langle H_i^s H_j^{s'} \rangle$ and $\langle K_i^s K_j^{s'}(t) \rangle$ will be functions of the distance between the sites i and j, and the correlation length will be of the order of the interaction radius. Since it is assumed that over this distance the macroscopic characteristics of the system change only slightly, one may expand $\beta^{s'}(\mathbf{x}_j)$ about the site i, as a result of which from (5) we find

$$\overline{K^s(\mathbf{x})} \simeq \sum_{ij}\sum_{s'} \delta(\mathbf{x}-\mathbf{x}_i) \times$$

$$\times \int_{-\infty}^{0} dt\, e^{\varepsilon t} \left\langle K_i^s K_j^{s'}(t) \right\rangle \frac{1}{2} (\mathbf{x}_i - \mathbf{x}_j)_\chi (\mathbf{x}_i - \mathbf{x}_j)_{\chi'} \nabla_\chi \nabla_{\chi'} \beta^{s'}(\mathbf{x}),$$

$$H^s(\mathbf{x}) = -\sum_{ij}\sum_{s'} \delta(\mathbf{x}-\mathbf{x}_i) \left\langle H_i^s H_j^{s'} \right\rangle \beta^{s'}(\mathbf{x}). \tag{6}$$

Assuming, as usual,

$$\left\langle K_i^s K_j^{s'}(t) \right\rangle = \left\langle K_i^s K_j^{s'} \right\rangle G(t)$$

and taking into account that in all the cases considered here

$$\left\langle H_i^s H_j^{s'} \right\rangle = \left\langle H_i^s H_j^s \right\rangle \delta_{ss'}, \qquad \left\langle K_i^s K_j^{s'} \right\rangle = \left\langle K_i^s K_j^s \right\rangle \delta_{ss'},$$

after substituting (6) into (3) (together with the assumption of quasistaticity of the process), we arrive at the diffusion equation for the inverse temperature of subsystem s:

$$\partial \beta^s(\mathbf{x}, t)/\partial t = D^{\chi\chi'} \nabla_\chi \nabla_{\chi'} \beta^s(\mathbf{x}, t), \tag{7}$$

where the tensor of the diffusion coefficient is determined by the expression

$$D^{\chi\chi'} = -\frac{\frac{1}{2}\sum_j (\mathbf{x}_i - \mathbf{x}_j)_\chi (\mathbf{x}_i - \mathbf{x}_j)_{\chi'} \int_{-\infty}^{0} dt\, e^{\varepsilon t} \left\langle K_i^s K_j^s(t) \right\rangle}{\sum_j \left\langle H_i^s H_j^s \right\rangle}. \tag{8}$$

Taking into account that $\langle K_i^s K_j^s(t)\rangle$ is an even function of $\mathbf{x}_i - \mathbf{x}_j$ and introducing the Fourier transform

$$\mathcal{K}_{xx'}(\omega) = \frac{1}{2\pi}\int dt\, e^{i\omega t} \frac{\sum_j (\mathbf{x}_i - \mathbf{x}_j)_x (\mathbf{x}_i - \mathbf{x}_j)_{x'} \langle K_i^s K_j^s(t)\rangle}{\sum_j (\mathbf{x}_i - \mathbf{x}_j)_x (\mathbf{x}_i - \mathbf{x}_j)_{x'} \langle K_i^s K_j^s\rangle},$$

from (8) we obtain

$$D^{xx'} = -\frac{\pi}{2}\frac{\sum_j (\mathbf{x}_i - \mathbf{x}_j)_x (\mathbf{x}_i - \mathbf{x}_j)_{x'} \langle K_i^s K_j^s\rangle}{\sum_j \langle H_i^s H_j^s\rangle}\mathcal{K}_{xx'}(\omega = 0). \tag{9}$$

If the correlator $\mathcal{K}_{xx'}(\omega)$ has a Gaussian form, then

$$\mathcal{K}_{xx'}(0) = (2\pi\mathcal{K}^{(2)}_{xx'})^{-1/2},$$

where

$$\mathcal{K}^{(2)}_{xx'} = -\frac{\sum_j (\mathbf{x}_i - \mathbf{x}_j)_x (\mathbf{x}_i - \mathbf{x}_j)_{x'} \langle [K_i^s H^s][K_j^s H^s]\rangle}{\sum_j (\mathbf{x}_i - \mathbf{x}_j)_x (\mathbf{x}_i - \mathbf{x}_j)_{x'} \langle K_i^s K_j^s\rangle}$$

is the second moment of the correlation function.

Then, in the case of cubic symmetry, from (9) we obtain an expression for the diffusion coefficient equivalent to the result of work (1). (In this connection one must bear in mind the Zeeman subsystem.)

If, however, the correlator has a Lorentzian form, then

$$\mathcal{K}_{xx'}(0) = \frac{1}{2\sqrt{3}}\frac{(\mathcal{K}^{(2)}_{xx'})^{3/2}}{(\mathcal{K}^{(4)}_{xx'})^{1/2}},$$

where

$$\mathcal{K}^{(4)}_{xx'} = -\frac{\sum_j (\mathbf{x}_i - \mathbf{x}_j)_x (\mathbf{x}_i - \mathbf{x}_j)_{x'} \langle [[K_i^s H^s]H^s][[K_i^s H^s]H^s]\rangle}{\sum_j (\mathbf{x}_i - \mathbf{x}_j)_x (\mathbf{x}_i - \mathbf{x}_j)_{x'} \langle K_i^s K_j^s\rangle}$$

is the fourth moment of the correlation function.

In this case the expression for the diffusion coefficient will have an entirely different behavior. Such a situation may occur when chaotically distributed impurities are present in the sample.

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Institute of Physics
Academy of Sciences of the Georgian SSR
Tbilisi

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Note: Figure translations are in progress. See original paper for figures.