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Abstract

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PHYSICS

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ON TAKING INTERACTION INTO ACCOUNT IN CONSTRUCTING A NONEQUILIBRIUM DENSITY MATRIX

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In constructing a stationary nonequilibrium density matrix ⁽¹⁾ for a macrosystem consisting of several weakly coupled subsystems, ambiguity may arise in the question of the proper account of the interaction \mathcal{H}' between the subsystems. Usually this interaction is assigned the temperature of one of the subsystems ⁽²⁾, or else it is noted that the final results do not depend on the assigned temperature β' so long as \mathcal{H}' can be regarded as a small perturbation ⁽³⁾.

In the stationary case the energy conservation law holds

$$\sum_{k=1}^n \frac{d\mathcal{H}_k}{dt} + \frac{d\mathcal{H}'}{dt} = 0, \quad (1)$$

where \mathcal{H}_k is the Hamiltonian of the k -th subsystem; $\frac{d\mathcal{H}_k}{dt} = \frac{1}{i}[\mathcal{H}_k, \mathcal{H}]$, $\mathcal{H} = \sum_k \mathcal{H}_k + \mathcal{H}'$ is the Hamiltonian of the system, and n is the number of subsystems.

It follows from (1) that when the system is divided into n subsystems only $n-1$ are independent. In considering concrete processes the interaction energy is often not included in the energy balance and, instead of (1), the approximate conservation law ^(3,4)

$$\sum_{k=1}^n \frac{d\mathcal{H}_k}{dt} \simeq 0 \quad (2)$$

is used. Thus the term $d\mathcal{H}'/dt$ is discarded; generally speaking, it is of the same order as the term $\sum_{k=1}^n d\mathcal{H}_k/dt$. It is not difficult to verify that, at least in the high-temperature approximation, neither β' nor $d\mathcal{H}'/dt$ in (1) contributes to the mean values

$$\overline{\mathcal{H}}_k = \text{Sp } \rho \mathcal{H}_k, \quad d\overline{\mathcal{H}}_k/dt = \text{Sp } \rho d\mathcal{H}_k/dt,$$

which are used in deriving equations for the inverse temperatures of the subsystems. But sometimes one has to calculate the mean values $\overline{A}_j = \text{Sp } \rho A_j$ of such quantities A_j that are proportional to \mathcal{H}' . In this case it is not evident in advance that the final result also will not depend on β' , and that the use of (2) is legitimate.

In the present note this question is discussed for the example of calculating the real part of the complex susceptibility χ for a spin system in external constant and alternating magnetic fields. The Hamiltonian of the system in the rotating coordinate system has the form

$$\mathcal{H} = \mathcal{H}_z + \mathcal{H}_d + \mathcal{H}_x, \quad \mathcal{H}_z = (\omega_0 - \omega)S_z, \quad \mathcal{H}_x = \omega_1 S_x, \quad (3)$$

where \mathcal{H}_d is the secular part of the dipole-dipole interaction of the spins; $\omega_0 = \gamma H_0$; $\omega_1 = \gamma H_1$; H_0 is the constant magnetic field; ω, H_1 are the frequency and semiamplitude of the alternating field; $S_\alpha = \sum_i S_{i\alpha}$, $\alpha = x, y, z$, are spin operators.

According to (1), we form the generalized integrals of motion

$$\begin{aligned} \widetilde{\mathcal{H}}_z &= \mathcal{H}_z - \int_{-\infty}^0 e^{\varepsilon t} \dot{\mathcal{H}}_z(t) dt, & \widetilde{\mathcal{H}}_d &= \mathcal{H}_d - \int_{-\infty}^0 e^{\varepsilon t} \dot{\mathcal{H}}_d(t) dt, \\ \widetilde{\mathcal{H}}_x &= \mathcal{H}_x - \int_{-\infty}^0 e^{\varepsilon t} \dot{\mathcal{H}}_x(t) dt = \mathcal{H}_x + \int_{-\infty}^0 e^{\varepsilon t} \{ \dot{\mathcal{H}}_x(t) + \dot{\mathcal{H}}_d(t) \} dt. \end{aligned} \quad (4)$$

Let us note that, in contrast to works ⁽²⁻⁴⁾, here \mathcal{H}_x is also introduced into the consideration. In the last expression (4) the exact conservation law has been used,

$$\dot{\mathcal{H}}_x = -\dot{\mathcal{H}}_z - \dot{\mathcal{H}}_d. \quad (5)$$

The quasiequilibrium density matrix in the high-temperature approximation has the form

$$\rho = \frac{1}{\text{Sp } 1} \left\{ 1 - \beta_z \mathcal{H}_z - \beta_d \mathcal{H}_d - \beta_x \mathcal{H}_x + (\beta_z - \beta_x) \int_{-\infty}^0 e^{\varepsilon t} \mathcal{H}_z(t) dt + (\beta_d - \beta_x) \int_{-\infty}^0 e^{\varepsilon t} \dot{\mathcal{H}}_d(t) dt \right\}, \quad (6)$$

where β_z and β_d are the inverse temperatures of the Zeeman subsystem and the dipole-dipole reservoir, and β_x is the inverse temperature assigned to the

invariant part of the interaction $\widetilde{\mathcal{H}}_x$. The time dependence of the operators denotes the Heisenberg representation.

Using the density matrix (6) and a phenomenological treatment of spin-lattice relaxation, analogously to ^(4,5), one easily obtains the equations

$$\begin{aligned}\frac{d\beta_z}{dt} &= -2W(\omega - \omega_0)(\beta_z - \beta_d) - \left(\beta_z - \frac{\omega_0}{\omega_0 - \omega} \beta_L \right) / T_z, \\ \frac{d\beta_d}{dt} &= -2W(\omega - \omega_0) \frac{(\omega_0 - \omega)^2}{\omega_d^2} (\beta_d - \beta_z) - \frac{\beta_d - \beta_L}{T_d}, \\ \frac{d\beta_x}{dt} &= -\frac{\beta_x - \beta_L}{T'_x} - \frac{\beta_x}{T''_x},\end{aligned}\quad (7)$$

where $W(\omega - \omega_0) = \frac{\pi\omega_1^2}{2} \varphi(\omega - \omega_0)$ is the usual probability of transitions induced by the alternating field; $\varphi(\omega - \omega_0)$ is the absorption line shape; $\omega_d^2 = \text{Sp } \mathcal{H}_d^2 / \text{Sp } S_z^2$; T_z and T_d are the times of spin-lattice relaxation of the Zeeman subsystem and the DDR; T'_x and T''_x are the relaxation times due respectively to the secular and nonsecular parts of the spin-lattice interaction ⁽⁶⁾; β_L is the inverse temperature of the lattice. It should be noted that the same equations for β_z and β_d are obtained also in the case when $\widetilde{\mathcal{H}}_x$ is not taken into account and, instead of (5), the approximate conservation law is used,

$$\dot{\mathcal{H}}_d + \dot{\mathcal{H}}_z = 0. \quad (8)$$

It follows from this that the inclusion of $\widetilde{\mathcal{H}}_x$ also does not change the imaginary part of the complex susceptibility χ'' . We shall now calculate χ' . We have ⁽⁵⁾

$$\chi' = M_x / 2H_1, \quad (9)$$

where M_x is the mean value of the x -th component of the magnetization in the rotating coordinate system, which in our case is equal to

$$M_x = \gamma \bar{S}_x = \gamma \text{Sp } \rho S_x. \quad (10)$$

With the aid of (6) and (10) we obtain ($\langle \dots \rangle \equiv \text{Sp}(\dots) / \text{Sp } 1$)

$$\begin{aligned}\bar{S}_x &= -\beta_x \omega_1 \langle S_x^2 \rangle + (\beta_z - \beta_x) \int_{-\infty}^0 e^{\varepsilon t} \langle S_x \dot{\mathcal{H}}_z(t) \rangle dt + \\ &+ (\beta_d - \beta_x) \int_{-\infty}^0 e^{\varepsilon t} \langle S_x \dot{\mathcal{H}}_d(t) \rangle dt.\end{aligned}\quad (11)$$

Evaluation of the integrals entering (12), to first order in \mathcal{H}_x , gives

$$\int_{-\infty}^0 e^{\varepsilon t} \langle S_x \dot{\mathcal{H}}_z(t) \rangle dt = \langle S_x^2 \rangle \omega_1 (\omega - \omega_0) J_1(\omega - \omega_0),$$

$$\int_{-\infty}^0 e^{\varepsilon t} \langle S_x \dot{\mathcal{H}}_d(t) \rangle dt = -\langle S_x^2 \rangle \omega_1 [1 + (\omega - \omega_0) J_1(\omega - \omega_0)], \quad (12)$$

$$J_1(x) = \int_{-\infty}^{\infty} \frac{\Phi(y) dy}{y - x} = -J_1(-x)$$

(the last integral $\int_{-\infty}^{\infty}$ is taken in the sense of the principal value).

For χ' we finally obtain

$$\chi' = \frac{1}{2} \chi_0 \left\{ (\omega - \omega_0) J_1(\omega - \omega_0) \frac{\beta_z - \beta_d}{\beta_L} - \frac{\beta_d}{\beta_L} \right\}, \quad (13)$$

where $\chi_0 = N \gamma^2 \langle S_z^2 \rangle \beta_L$ is the static susceptibility. Thus, the terms with β_x do not enter into χ' , so that assigning a separate temperature to the interaction \mathcal{H}_x , or arbitrarily including it in any of the subsystems, does not affect the final result. However, the use of the approximate expression (8) instead of the exact one (5) proves to be incorrect in finding χ' , since in this case the last term in (13) is lost.

The example considered shows that, at least in the lowest order of perturbation theory, taking account of the invariant part of the interaction \mathcal{H}' in constructing the nonequilibrium density matrix does not affect the expressions for χ'_x and χ''_x . At the same time, the use of the approximate conservation law (2) may prove to be incorrect in calculating quantities proportional to the perturbation \mathcal{H}' , as occurs for χ' . This latter circumstance must be taken into account when considering specific problems.

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