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ON THE ADIABATIC APPROXIMATION FOR THE DENSITY MATRIX OF AN ISOLATED SPIN SYSTEM

A. A. SAMOKHIN

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We obtain an expression for the adiabatic response of a paramagnetic spin-system without using the quasi-equilibrium form of the density matrix.

THE behavior of an isolated spin-system with a Hamiltonian containing a dipole-dipole and a Zeeman energy, $\hat{\mathscr{H}}(t) = \hat{\mathscr{H}}_0 - \hat{M}h(t)$, in a variable magnetic field $h(t)$ is in the adiabatic approximation determined by a density matrix of the form

$$\rho(t) = \exp[-\alpha(t)\hat{\mathscr{H}}(t)] / \operatorname{Sp}\exp[-\alpha\hat{\mathscr{H}}], \qquad (1)^*$$

where the time dependence of $\alpha(t)$ can be found from the equation

$$\operatorname{Sp}\hat{\mathscr{H}}\partial\rho/\partial t = 0. \qquad (2)$$

In the high-temperature approximation $\rho(t) \approx [I - \alpha(t)\hat{\mathscr{H}}(t)/\operatorname{Tr} I$, and it follows from (1) and (2) that we have for the magnetic moment

$$\operatorname{Sp}\hat{M}\rho(t) = \chi_0 h(t)[1 + h^2(t)/H^2]^{-1/2}, \qquad (3)$$

where $\chi_0 = \alpha_0 \operatorname{Tr}\hat{M}^2/\operatorname{Tr} I$, $H^2 = \operatorname{Tr}\hat{\mathscr{H}}_0^2/\operatorname{Tr}\hat{M}^2$ and where we have assumed for the sake of simplicity that the operator $\hat{M}$ (we denote here by $\hat{M}$ the z-component of the magnetic moment) has no diagonal part in the representation which diagonalizes the unperturbed Hamiltonian $\hat{\mathscr{H}}_0$.

In the present paper we consider the adiabatic approximation in the framework of non-stationary perturbation theory for the density matrix of an isolated system. Such a procedure enables us to obtain an expression for the magnetic moment (3) directly from the quantum-mechanical Liouville equation without assuming beforehand the form of the density matrix (1): The following relation for the diagonal parts $\hat{A}_0$ and $\hat{B}_0$ of macroscopic operators $\hat{A}$ and $\hat{B}$ will then play an essential part:

$$\operatorname{Sp}\hat{A}_0\hat{B}_0 = \operatorname{Sp}(\hat{A}\hat{\mathscr{H}}_0)\operatorname{Sp}(\hat{B}\hat{\mathscr{H}}_0)/\operatorname{Sp}\hat{\mathscr{H}}_0^2, \qquad (4)$$

which expresses the equality of the so-called isolated and adiabatic susceptibilities.[1]

Considering $-\hat{M}h(t)$ as a perturbation, solving the Liouville equation by iteration $\rho(t) = \rho^{(0)} + \ldots \rho^{(n)} + \ldots$ with the initial condition $\rho(0) = \rho^{(0)} = [1 - \alpha_0\hat{\mathscr{H}}_0]/\operatorname{Tr} I$ and $h(0) = 0$, we get for $M^{(n)}$

$$M^{(n)} = \operatorname{Sp}\hat{M}\rho^{(n)} = \frac{\alpha_0(-1)^n}{\operatorname{Sp} I}\int_0^t dt_1\ldots \times \int_0^{t_{n-1}} dt_n h(t_1)\ldots h(t_{n-1})\frac{dh(t_n)}{dt_n} \times \operatorname{Sp}\{\hat{F}^{(n-1)}(t, t_1\ldots t_n)\hat{M}(t_n)\},$$

$$\hat{F}^{(n-1)} = [\ldots[\hat{M}(t), \hat{M}(t_1)]\ldots\hat{M}(t_{n-1})](i\hbar)^{1-n}, \quad \times\ d\hat{M}(t)/dt = [\hat{M}, \hat{\mathscr{H}}_0]/i\hbar. \qquad (5)$$

Writing $\operatorname{Tr}\hat{F}^{(n-1)}\hat{M}(t_n)$ as a sum of traces of products of diagonal and non-diagonal operators,

$$i\hbar\operatorname{Sp}\hat{F}^{(n-1)}\hat{M}(t_n) = \operatorname{Sp}\{\hat{F}_0^{(n-2)}[\hat{M}(t_{n-1}), \hat{M}(t_n)]_0\} + \operatorname{Sp}\{\hat{F}_I^{(n-2)}[\hat{M}(t_{n-1}), \hat{M}(t_n)]_I\}, \qquad (6)$$

we note that the second term contains at least a ternary correlation function[2] and can thus be dropped in the adiabatic approximation. Using (4) we then get from (6)

$$\operatorname{Sp}\hat{F}^{(n-1)}\hat{M}(t_n) \approx \frac{1}{H^2}\operatorname{Sp}\left\{\hat{F}^{(n-3)}\frac{d\hat{M}(t_{n-2})}{dt_{n-2}}\right\}\frac{d}{dt_n}\varphi(t_n - t_{n-1});$$

$$\varphi(t_n - t_{n-1}) = \operatorname{Sp}\hat{M}(t_n)\hat{M}(t_{n-1})/\operatorname{Sp}\hat{M}^2 \qquad (7)$$

and integration by parts gives for $M^{(n)}$

$$M^{(n)} \approx \frac{\alpha_0(-1)^{n-1}}{\operatorname{Sp} I}\frac{3}{2H^2}\int_0^t dt_1\ldots \times \int_0^{t_{n-3}} dt_{n-2} h(t_1)\ldots h^2(t_{n-2})\frac{dh(t_{n-2})}{dt_{n-2}} \times \operatorname{Sp}\{\hat{F}^{(n-3)}\hat{M}(t_{n-2})\}. \qquad (8)$$

*Sp ≡ Tr.

We dropped in (8) a term containing the expression

$$\varphi(t_{n-1})\frac{dh}{dt}\Big|_0 + \int_0^{t_{n-1}} dt_n \frac{d^2h(t_n)}{dt_n^2}\varphi(t_n - t_{n-1}),$$

which also gives no contribution to $M^{(n)}$ in the adiabatic approximation. Continuing this process we have finally for $M_{ad}^{(n)}$

$$M_{ad}{}^{(n)} = \chi_0 h(t)(-1)^{k+1}\frac{1\cdot3\cdot5\ldots(2k+1)}{2^{k+1}(k+1)!}\left(\frac{h^2(t)}{H^2}\right)^{k+1},$$

$$n = 2k+3, \quad k = 0, 1, 2\ldots, \tag{9}$$

which corresponds to (3).

The adiabatic approximation is valid for sufficiently low frequencies of the variable field $\omega t < 1$ and for not too large times, $t < H^2/h^2\omega^2\tau$ for systems such that statistical equilibrium can be established by means of internal interactions. The relaxation time in such a system is determined by the following equation

$$\tau = \int_{-\infty}^{0} dt\, \varphi(t).$$

The terms omitted when we derived the adiabatic response contain correlation functions of different order and different powers in ω and t. They characterize the deviation of the system from internal equilibrium with respect to the instantaneous value of the total Hamiltonian $\hat{\mathcal{H}}(t)$. Taking these terms into account enables us to find an expression for the non-adiabatic response of an isolated system.

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[1] J. A. Tjon, Physica **30**, 1341 (1964).
[2] A. A. Samokhin, Physica **32**, 823 (1966).

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