THE NONLINEAR THEORY OF A SPIN SYSTEM'S REACTION ON AN EXTERNAL PERTURBATION

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Received 12 January 1975

The line shape of magnetic resonance absorption is calculated by the nonlinear theory of irreversible processes.

The theoretical investigation of the magnetic resonance (MR) phenomenon based on the linear theory of irreversible processes [1,2] shows that the absorption line shape is defined by interactions within a magnetic system but does not depend on the intensity of variable,magnetic field, that is the linear theory does not describe a saturation effect. The proposed theory of nonlinear theory does not describe a saturation effect. The proposed theory of nonlinear response describes the saturation of MR.

Suppose that the unperturbed Hamiltonian of the spin system is $\mathcal{H}_0$, and the Hamiltonian of the interaction of the spin system with an external variable magnetic field is $\mathcal{H}(t)$. Then the density matrix of the system obeys the equation of motion:

$$\frac{\mathrm{d}}{\mathrm{d}t}\rho(t) = \frac{1}{\mathrm{i}\hbar}[\mathcal{H}_0 + \mathcal{H}(t), \rho(t)] \ . \tag{1}$$

The density matrix may be represented as $\rho(t) = \rho_0 + \Delta\rho(t)$, where ρ_0 means the density matrix of the system in the thermodynamic equilibrium state. Substituting $\rho(t)$ for eq. (1) we obtain:

$$\frac{\mathrm{d}}{\mathrm{d}t}\Delta\rho(t) = \frac{1}{\mathrm{i}\hbar}[\mathcal{H}(t), \rho_0] + \frac{1}{\mathrm{i}\hbar}[\mathcal{H}_0 + \mathcal{H}(t), \Delta\rho(t)] \ . \tag{2}$$

In contrast to [2] we do not omit the nonlinear term $[\mathcal{H}(t), \Delta\rho(t)]/\mathrm{i}\hbar$ in eq. (2). Assume that our system has been in equilibrium at $t = -\infty$ with the unperturbed Hamiltonian $\mathcal{H}_0$ and that the variable magnetic field has been switched on adiabatically at $t = -\infty$, that is $\rho(-\infty) = \rho_0$ and $\mathcal{H}(-\infty) = 0$. Then the solution of eq. (2) under the initial condition $\Delta\rho(-\infty) = 0$ is:

$$\Delta\rho(t) = \frac{1}{\mathrm{i}\hbar}\int_{-\infty}^{t}\mathrm{d}t' \exp\left\{\frac{1}{\mathrm{i}\hbar}\int_{t'}^{t}(\mathcal{H}(\tau) + \mathcal{H}_0)\,\mathrm{d}\tau\right\}[\mathcal{H}(t'), \rho_0]\exp\left\{-\frac{1}{\mathrm{i}\hbar}\int_{t'}^{t}(\mathcal{H}(\tau) + \mathcal{H}_0)\,\mathrm{d}\tau\right\} . \tag{3}$$

The expectation value of the magnetic moment operator $\boldsymbol{M}$ will be

$$\langle \boldsymbol{M}(t)\rangle = \mathrm{Sp}(\rho(t)\boldsymbol{M}) = \mathrm{Sp}(\rho_0\boldsymbol{M}) + \frac{1}{\mathrm{i}\hbar}\int_{-\infty}^{t}\mathrm{d}t'\,\mathrm{Sp}\Bigg([\mathcal{H}(t'), \rho_0] \times \exp\left\{-\frac{1}{\mathrm{i}\hbar}\int_{t'}^{t}(\mathcal{H}(\tau) + \mathcal{H}_0)\,\mathrm{d}\tau\right\}\boldsymbol{M}\exp\left\{\frac{1}{\mathrm{i}\hbar}\int_{t'}^{t}(\mathcal{H}(\tau) + \mathcal{H}_0)\,\mathrm{d}\tau\right\}\Bigg) . \tag{4}$$

Let us present the Hamiltonian of the system in the form $\mathcal{H}_0 = \mathcal{H}_1 + \mathcal{H}_2 + \mathcal{H}'$, where $\mathcal{H}_1$ is the Hamiltonian of Zeeman interaction of magnetic system in a constant magnetic field H_z, $\mathcal{H}_2$ is the Hamiltonian of molecular degrees of freedom (the "lattice" variables), $\mathcal{H}'$ is the Hamiltonian of dipole-dipole interaction. Let us assume that the energy of $\mathcal{H}_1 + \mathcal{H}_2$ is much larger than $\mathcal{H}(\tau) + \mathcal{H}'$. Applying Feynman's operator calculus [3], eq. (3) may be expressed as a power series in $(\mathcal{H}(\tau) + \mathcal{H}')$ up to the second power. Using the results