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Kyoto University
Quantum Decoherence of a Spin System
Strongly Coupled to a Quantum Environment

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Abstract

Quantum theoretical relaxation and strongly interacting spin systems have been applied to analyze experimental results of the NMR and \( \mu \)SR (muon spin resonance / relaxation / rotation). Especially, the model that describes the interaction between the relevant spin and the environment as a stochastic process has been found useful because the model can provide the systematic examination on effects due to arbitrary modulation speed of the fluctuating field exerted from the environment[1, 2, 3, 4, 5, 6]. On the other hand, quantum effects of the environment have not enjoyed due interest for more systematic examination.

The objective in this paper is to examine quantum effects of the environment by using a projection operator method for dynamical variables[7, 8]. The time dependence of a relevant spin is described with a convolution type of integrals up to infinite orders[9]. Using Laplace transform, we have obtained a spectrum in a continued fraction form, which enables us to take into account the strong coupling between the spin and the environment.

This paper is constructed as follows: In section 2, preliminaries for obtaining a basic equation is reviewed. The method is applied to the case where a spin interacts with a
quantum environment in section 3. Magnetic susceptibility is obtained in a continued
fraction form in section 4. Section 5 provides concluding remarks.

2 Preliminaries

Let us consider the system which consists of the unperturbed part Hamiltonian \( \mathcal{H}_0 \) and
the perturbation part \( \mathcal{H}_1(t) \):

\[
\mathcal{H}(t) = \mathcal{H}_0 + \mathcal{H}_1(t),
\]

with

\[
\mathcal{H}_0 = \mathcal{H}_S + \mathcal{H}_B.
\]

For later use, we confine ourselves the relevant system to a \( \frac{1}{2} \)-spin \( \mathcal{H}_S \equiv h\omega_0 S_z \) where
\( S_z \) is a z-component of a spin operator and we examine the time dependence of the
transverse component \( S_+(t) \equiv S_x(t) + iS_y(t) \). In \( \mathcal{H}_B \), \( \mathcal{H}_B \) indicates the Hamiltonian of
an environment.

In order to determine the time evolution of the relevant system under the interaction
with the environment, we use a projection operator \( P \) which satisfies an idempotent
relation, \( P^2 = P \), and an operator \( Q(= 1 - P) \). For an operator \( \hat{S}_+(t) \) in an interaction
picture defined as

\[
\hat{S}_+(t) \equiv e^{-i\omega(t-t_0)}S_+(t),
\]

we find

\[
\frac{d}{dt}\hat{S}_+(t) = \hat{U}_-(t,t_0)\mathcal{P}i\hat{L}_1(t)S_+ + \int_{t_0}^{t}d\tau K(t,\tau)S_+ + I(t)S_+ .
\]

where we use the following definitions:

\[
K(t,\tau) = \hat{U}_-(\tau,t_0)\mathcal{P}i\hat{L}_1(\tau)\mathcal{Q}\hat{u}_-(t,\tau)i\hat{L}_1(t),
\]

\[
I(t) = \mathcal{Q}\hat{u}_-(t,t_0)i\hat{L}_1(t),
\]

with

\[
\hat{U}_-(t,t_0) \equiv T_-[e^{i\int_{t_0}^{t}d\tau i\hat{L}_1(\tau)}],
\]

\[
\hat{u}_-(t,\tau) = T_-[e^{i\int_{t}^{\tau}d\tau' i\hat{L}_1(\tau')}Q].
\]
In eq.(2.8), the symbol $T_-$ indicates an increasing time ordering from the left to the right and

$$\hat{L}_1(t) = e^{i\mathcal{L}_1(t-t_0)} L_1(t) e^{-i\mathcal{L}_1(t-t_0)},$$

where $\mathcal{L}_\mu$ ($\mu = 0$ or 1) is the Liouville operator defined as

$$\mathcal{L}_\mu : = \frac{1}{\hbar} [\mathcal{H}_\mu, \cdot].$$

When we apply the basic equation (2.4) to actual systems, we have to evaluate the integrand $K(t, \tau)$ and the inhomogeneous term $I(t)$ which include ordered exponential expanded up to infinite orders. For example, the term including $K(t, \tau)$ is expanded as

$$\int_{t_0}^{t} d\tau \hat{K}_-(t, \tau) = \int_{t_0}^{t} dt_1 \hat{U}_-(t_1, t_0) \langle i\hat{L}_1(t_1) i\hat{L}_1(t) \rangle_{a.p.c.}$$

$$+ \sum_{n=3}^{\infty} \int_{t_0}^{t} dt_1 \int_{t_0}^{t_1} dt_2 \cdots \int_{t_0}^{t_{n-1}} dt_{n-1}$$

$$\times \hat{U}_-(t_{n-1}, t_0) \langle i\hat{L}_1(t_{n-1}) i\hat{L}_1(t_{n-2}) \cdots i\hat{L}_1(t) \rangle_{a.p.c.},$$

where we called the each order integrands " anti partial cumulants" which is defined as

$$\langle i\hat{L}_1(t_{n-1}) i\hat{L}_1(t_{n-2}) \cdots i\hat{L}_1(t) \rangle_{a.p.c.} \equiv \mathcal{P} i\hat{L}_1(t_{n-1}) Q_i \hat{L}_1(t_{n-2}) \cdots Q_i \hat{L}_1(t), \ (n \geq 2).$$

3 Basic Equation

Let us consider a spin system interacting with a quantum environment non-adiabatically:

$$\mathcal{H}_0 = \hbar \omega_0 S_z + \mathcal{H}_B,$$

$$\mathcal{H}_1 = \hbar (\omega_- S_+ + \omega_+ S_-),$$

where $\mathcal{H}_B$ indicates the Hamiltonian of the reservoir and $\omega_\pm$ are the reservoir operators. We assume the reservoir to be a collection of harmonic oscillators and define $\mathcal{H}_B$ and $\omega_\pm$ as

$$\mathcal{H}_B = \sum_j \hbar \omega_j b_j^\dagger b_j,$$

$$\omega_- \equiv \sum_j \kappa_j b_j \equiv (\omega_+)^\dagger,$$
where $b_j$ ($b_j^\dagger$) is an annihilation (creation) operator of the $j$-th oscillator and $\kappa_j$ is the coupling constant between the relevant spin and the $j$-th oscillator.

Now we apply (2.4) to this system by using the projection operator $\mathcal{P}$ defined as

$$\mathcal{P} \cdot \equiv \text{tr}_B \rho_B \cdot \equiv \langle \cdot \rangle_B , \quad (3.5)$$

where $\text{tr}_B$ indicates the trace operation for the reservoir ($B$) variables and

$$\rho_B \equiv \frac{e^{-\beta H_B}}{Z_B} , \quad (3.6)$$

$Z_B$ being the partition function; $\beta = \frac{1}{k_B T}$ where $k_B$ is the Boltzmann constant and $T$ is the temperature of the reservoir.

The operator $\hat{\mathcal{L}}_1(t)$ is written by

$$\hat{\mathcal{L}}_1(t) \cdot = [\tilde{\omega}_-(t) S_+ + \tilde{\omega}_+(t) S_- , \cdot ] , \quad (3.7)$$

with

$$\tilde{\omega}_+(t) = \sum_j e^{-i(\omega_0 - \omega_j) t} \kappa_j b_j \equiv \tilde{\omega}_-(t)^\dagger . \quad (3.8)$$

In order to evaluate the cumulants explicitly, we introduce a frequency distribution $\rho(\omega)$ of the coupling strength $\kappa_j$. We define the distribution by

$$\rho(\omega) \equiv \sum_j |\kappa_j|^2 \delta(\omega - \omega_j) \equiv \frac{\gamma}{\pi} \frac{\Delta^2}{(\omega - \omega_b)^2 + \gamma^2} , \quad (3.9)$$

assuming the distribution to be a Lorentzian with width $\gamma$, centered at $\omega_b$. Then, the correlation functions of the reservoir variable are found to be

\[
\langle \tilde{\omega}_+(t) \tilde{\omega}_-(t_1) \rangle_B = \sum_j |\kappa_j|^2 e^{-i(\omega_0 - \omega_j)(t-t_1)} n(\omega_j)
\]

\[
\approx \Delta^2 e^{-i(\omega_0 - \omega_b)(t-t_1) - \gamma |t-t_1|} n(\omega_b) . \quad (3.10)
\]

In obtaining (3.10), we defined $n(\omega_j)$ as

$$\langle \hat{b}_j^\dagger \hat{b}_j \rangle_B = \frac{1}{e^{\lambda_j} - 1} \equiv n(\omega_j) , \quad (3.11)$$

with

$$\lambda_j \equiv \beta \hbar \omega_j . \quad (3.12)$$
and assumed that the average number \( n(\omega_j) \) is assumed to be constant around the frequency range where \( \rho(\omega) \) changes appreciably. Correspondingly, we obtain the correlation function of inversed order as

\[
\langle \tilde{\omega}_-(t)\tilde{\omega}_+(t_1) \rangle_B = \sum_j |\kappa_j|^2 e^{i(\omega_0 - \omega_j)(t-t_1)}\bar{n}(\omega_j) \\
\cong \Delta^2 e^{i(\omega_0 - \omega_b)(t-t_1) - \gamma|t-t_1|n(\omega_b)},
\]

where

\[
\langle b_j b_j \rangle_B = 1 + \langle b_j^2 \rangle_B = \frac{1}{1 - e^{-\gamma_j}} \equiv \bar{n}(\omega_j),
\]

For higher order correlation functions, we have

\[
\langle \varphi_1 \varphi_2 \cdots \varphi_n \rangle_B = \langle \varphi_1 \varphi_2 \rangle_B \langle \varphi_3 \cdots \varphi_n \rangle_B + \langle \varphi_1 \varphi_3 \rangle_B \langle \varphi_2 \cdots \varphi_n \rangle_B + \cdots + \langle \varphi_1 \varphi_n \rangle_B \langle \varphi_2 \varphi_3 \cdots \varphi_{n-1} \rangle_B, \quad (n \geq 3)
\]

where

\[
\varphi_n \equiv \tilde{\omega}_+(t_n), \text{ or } \tilde{\omega}_-(t_n).
\]

Using (3.15) repeatedly, we have the theorem due to (Wick -) Bloch - de Dominicis. The odd order correlation disappear:

\[
\langle \varphi_1 \varphi_2 \cdots \varphi_n \rangle_B = 0, \quad (\text{for odd } n),
\]

since

\[
\langle \tilde{\omega}_\pm(t) \rangle_B = 0.
\]

The time evolution of \( \dot{\tilde{S}}_+(t) \) is given in the form of convolution-type integrals:

\[
\frac{d}{dt} \dot{\tilde{S}}_+(t) = -\Delta^2(n(\omega_b) + \bar{n}(\omega_b)) \int_0^t dt_1 \Xi_2(t, t_1)\dot{\tilde{S}}_+(t_1) \\
+ \Delta^4 n(\omega_b)\bar{n}(\omega_b) \int_0^t dt_1 \int_0^{t_1} dt_2 \int_0^{t_2} dt_3 \Xi_4(t, t_1, t_2, t_3)\dot{\tilde{S}}_+(t_3) \\
- \Delta^6 n(\omega_b)\bar{n}(\omega_b)(n(\omega_b) + \bar{n}(\omega_b)) \\
\times \int_0^t dt_1 \int_0^{t_1} dt_2 \int_0^{t_2} dt_3 \int_0^{t_3} dt_4 \int_0^{t_4} dt_5 \Xi_6(t, t_1, t_2, t_3, t_4, t_5)\dot{\tilde{S}}_+(t_5) \\
+ \cdots + \dot{\tilde{J}}_-(t),
\]

\[\text{(3.19)}\]
with

$$\Xi_2(t,t_1) = -\Delta^2 \xi_1(t-t_1)\eta_1(t-t_1) \, , (3.20)$$

$$\Xi_4(t,t_1,t_2,t_3) = \Delta^4 \xi_1(t-t_1)\xi_2(t_1-t_2)\xi_1(t_2-t_3) \times (2\eta_1(t-t_1)\eta_2(t_1-t_2)\eta_1(t_2-t_3) + \eta_1(t-t_1)\eta_1(t_2-t_3)) \, , (3.21)$$

$$\Xi_6(t,t_1,\ldots,t_5) = -\Delta^6 \{\xi_1(t-t_1)\xi_2(t_1-t_2)\xi_1(t_2-t_3)\xi_2(t_3-t_4)\xi_1(t_4-t_5)$$

$$\times (4\eta_1(t-t_1)\eta_2(t_1-t_2)\eta_1(t_2-t_3)\eta_2(t_3-t_4)\eta_1(t_4-t_5)$$

$$+ 2\eta_1(t-t_1)\eta_1(t_2-t_3)\eta_2(t_3-t_4)\eta_1(t_4-t_5)$$

$$+ 2\eta_1(t-t_1)\eta_2(t_1-t_2)\eta_1(t_2-t_3)\eta_1(t_4-t_5)$$

$$+ \eta_1(t-t_1)\eta_1(t_2-t_3)\eta_1(t_4-t_5))$$

$$+ \xi_1(t-t_1)\xi_2(t_1-t_2)\xi_3(t_2-t_3)\xi_2(t_3-t_4)\xi_1(t_4-t_5)$$

$$\times (2\eta_1(t-t_1)\eta_2(t_1-t_2)\eta_1(t_2-t_3)\eta_2(t_3-t_4)\eta_1(t_4-t_5)$$

$$+ 2\eta_1(t-t_1)\eta_1(t_2-t_3)\eta_2(t_3-t_4)\eta_1(t_4-t_5)$$

$$+ 2\eta_1(t-t_1)\eta_2(t_2-t_3)\eta_1(t_3-t_4)\eta_1(t_4-t_5)$$

$$+ 2\eta_1(t-t_1)\eta_1(t_2-t_3)\eta_1(t_4-t_5))$$

$$+ 2\eta_1(t-t_1)\eta_1(t_2-t_3)\eta_1(t_4-t_5))) \, , (3.22)$$

$$\Xi_{2n+1}(t,t_1,\ldots,t_{2n}) = 0 \ (\text{for } n \geq 1) \, , (3.23)$$

where we have defined

$$\xi_n(t) \equiv e^{-n\gamma t} \, , (3.24)$$

$$\eta_n(t) \equiv e^{-n(\omega_0-\omega)t} \, . (3.25)$$

\(\hat{J}(-t)\) in (3.19) is written by

$$\hat{J}(-t) \equiv Q\hat{u}(-t,t_0)i\hat{L}_1(t)S_+$$

$$= \sum_n \{\phi_{2n-1}(t) + \psi_{z,2n-1}(t)S_z + \psi_{-2n}(t)S_- + \psi_{+,2n}(t)S_+ \} \, . (3.26)$$

We can also explicitly determine the lower order terms of (3.26) as

$$\phi_1(t) = 0 \, , (3.27)$$

$$\psi_{z,1}(t) = -2i\tilde{\omega}_+(t) \, , (3.28)$$

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Thus, $\tilde{S}_+(t)$ can be determined by successive evaluation of the anti-partial cumulants.

\section{Magnetic Susceptibility}

Now we consider the magnetic susceptibility for a magnetic field in circulating polarization. The magnetic susceptibility $\chi_{+-}(\omega)$ is given by \cite{10}

\begin{equation}
\chi_{+-}(\omega) = \lim_{\epsilon \to 0} \int_0^\infty dt e^{-i\omega t - \epsilon} \Phi_{+-}(t),
\end{equation}

where

\begin{equation}
\Phi_{+-}(t) = \frac{i}{\hbar} \langle [S_+(t), S_-] \rangle
\end{equation}

is the response function. In (4.1), we exclude the multiplicative factor due to the gyromagnetic ratio.

With the use of the definition of the Fourier-Laplace transform, the magnetic susceptibility is written in the form

\begin{equation}
\chi_{+-}(\omega) = \frac{i}{\hbar} \langle [S_+[i\omega], S_-] \rangle,
\end{equation}

The Fourier-Laplace transform of the relation (3.19) is given by

\begin{equation}
S_+[i\omega] = \hat{S}_+[i(\omega - \omega_0)] = \frac{S_+ + \hat{J}_-[i(\omega - \omega_0)]}{i(\omega - \omega_0) - i\Sigma_+(\omega - \omega_0)},
\end{equation}

where

\begin{equation}
\hat{J}_-[i\omega] = \sum_n \{ \phi_{2n-1}[i\omega] + \psi_{2,2n-1}[i\omega]S_x + \psi_{-,2n}[i\omega]S_- + \psi_{+,2n}[i\omega]S_+ \}
\end{equation}

We can rearrange $\Sigma_+[i(\omega - \omega_0)]$ in (4.4) in the form of a continued fraction:

\[
\Sigma_+[i(\omega - \omega_0)] = \frac{\bar{n}(\omega_0) - n(\omega_0)}{n(\omega_0) + \bar{n}(\omega_0)\Delta^2\tilde{a}_1}
\]
\begin{align}
\frac{\bar{u}_1^{-1} - b\Delta^2 \bar{w}_2}{(\bar{v}_2 + \bar{w}_2)^{-1} - \frac{2b\Delta^2}{\bar{u}_3^{-1} + b\Delta^2(\bar{w}_2 - a\bar{w}_4) - a\Delta^2\bar{w}_4}} &= \frac{2b\Delta^2}{(\bar{v}_4 + \bar{w}_4)^{-1} - \cdots}, \\
\left. \right. \\
\text{with} \\
\bar{u}_n &= \frac{1}{(\omega - \omega_b - in\gamma)}, \\
\bar{v}_n &= \frac{1}{(\omega - \omega_b - in\gamma)}, \\
\bar{w}_n &= \frac{1}{(\omega - \omega_b) + (\omega_0 - \omega_b) - in\gamma}, \\
\text{where} \\
a &= \frac{4n(\omega_b)\bar{n}(\omega_b)}{(n(\omega_b) + \bar{n}(\omega_b))^2}, \\
b &= n(\omega_b) + \bar{n}(\omega_b). \\
\text{The magnetic susceptibility is given by} \\
\chi_{\pm}(\omega) &= \frac{i}{\hbar} \frac{2}{i(\omega - \omega_0) - i\Sigma_+[i(\omega - \omega_0)]} \langle S_z \rangle. \\
\text{In obtaining (4.12), we assumed a decoupled initial density matrix } W(0), \text{ i.e., } W(0) = \\
\rho_s \otimes \rho_B \text{ where } \rho_s \rho_B \text{ is the initial density matrix of the spin system (the reservoir).} \\
\text{At } T \sim 0, \text{ virtual excitation of energy quanta is expected to be within single particle states, and thus we have only to retain the second order term in } \Sigma_+[i(\omega - \omega_0)]. \text{ The magnetic susceptibility reduces to} \\
\chi_{\pm}(\omega) &= \frac{i}{\hbar} \frac{2}{i(\omega - \omega_0) - i\Delta^2\bar{u}_1} \langle S_z \rangle, \\
\text{In the opposite limit of high temperature limit, (4.6) is written as} \\
\Sigma_+[i(\omega - \omega_0)] &= \frac{\Delta^2}{\bar{u}_1^{-1} - \Delta^2 \bar{w}_2 - \frac{\Delta^2}{(\bar{v}_2 + \bar{w}_2)^{-1} - \frac{2\Delta^2}{\bar{u}_3^{-1} + \Delta^2(\bar{w}_2 - \bar{w}_4) - \frac{2\Delta^2}{(\bar{v}_4 + \bar{w}_4)^{-1} - \cdots}}}}. \\
\end{align}
Figure 1: Frequency dependence of $\text{Im}[\chi_+(\omega')] / 2 \langle S_z \rangle$ for $\lambda = 1, \omega_0 = 10, \omega_b = 10$. The interaction strength $\alpha$ is changed from 0.1 to 100.

which coincides with the result obtained for the stochastic environmental fields by Shibata and Sato\cite{5}. Thus the magnetic susceptibility (4.12) can be used for the temperature effects ranging from zero to high temperature. For finite temperatures, the continued fraction effectively converges in certain finite orders corresponding to the system parameters.

In fig. 1, we show frequency dependence of $\text{Im}[\chi_+(\omega')] / 2 \langle S_z \rangle$ for relatively low temperature $\lambda(=\hbar \omega_b / k_B T = 1)$, where the variable of abscissa is scaled as $\omega' = \omega / (\sqrt{2}\Delta)$. The interaction strength $\alpha(=\sqrt{2}\Delta / \gamma)$ is changed from 0.1 to 100. As the interaction strength becomes larger, the line shapes changed from a single peak to two peaks.

5 Concluding remarks

In this paper, we obtained the magnetic susceptibility of a spin system in non-adiabatic contact with a quantum environment. The basic equation for the system operator $S^\dagger(t)$ is obtained by successive evaluation of the anti-partial cumulants. With the use of the basic equation, we could express the magnetic susceptibility in continued-fraction form which takes into account the interaction between the spin and the environment up to infinite orders.

As the $\frac{1}{2}$ spin system is equivalent to a two-level system, the model treated in this paper also describes relaxation phenomena of a dissipative two-level system. Since a proposal of
“spin-boson” model[11], it has attracted considerable attention. This model can be used to examine the macroscopic quantum tunneling (MQT) phenomena in a SQUID[12, 13], the quantum nucleation in the mixture of $He^3$ and $He^4[14]$, etc. Rotating the coordinate system of the Hamiltonian (3.1) $\sim$ (3.3), we can obtain the same Hamiltonian as that of the “spin-boson” model. Thus, when we evaluate $\langle S_+(t) \rangle$ using the inverse Laplace Fourier transform, we can discuss the dynamics of the “spin-boson” model.

References


