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LOCAL STOCHASTIC MODELS IN LARGE-SCALE STOCHASTIC HAMILTONIAN SYSTEMS*

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ABSTRACT

We consider the problem of isolating the dynamical behavior of a portion of a system imbedded in a large stochastic system. The large scale system is assumed to have a Hamiltonian structure. The method employed is the derivation of the appropriate master equations. Several examples illustrate the theory.

1. A Probabilistic Mechanism for Dynamic Instabilities

The equations

$$M_k\frac{d^2\delta_k(t)}{dt^2}+d_k\frac{d\tilde{\delta}_k(t)}{dt}=P_{mk}-E_k{}^2G_{kk} - \sum_{j=1}^{n}E_kE_jB_{kj}\sin[\tilde{\delta}_k(t)-\tilde{\delta}_j(t)] \quad (1.1)$$

$$\tilde{\delta}_k(0), d\tilde{\delta}_k(0)/dt \text{ given, } t\geqq 0,\ k=1,2,\ldots,n$$

describe the dynamics of an electric power network composed of n synchronous machines interconnected via an admittance network. Here M_k is the angular momentum, d_k the constant damping, P_{mk} the mechanical power input(constant) G_{kk} the internal conductance, E_k the magnitude of the machine internal voltage, B_{kj} the transfer susceptance of the transmission network, and $\delta_k(t)$ is the rotor angle of the machine relative to a synchronous frame. In the model (1.1) system loads have been represented as impedances and imbedded in B_{kj}. The problem of interest is the explanation of "spontaneously generated" small signal instabilities, called dynamic instabilities, observed in unfaulted electrical power systems [1]. While these phenomena have many causes, the model (1.1) is capable of producing an effect of this general type which is unknown to power engineers.

To present the result, it is convenient to change coordinates in (1.1). We define $M=\sum_{k=1}^{n}M_k$, $\delta_0(t)=(\sum_{k=1}^{n}M_k\delta_k(t))/M$, the "center of angle." We may, without loss of generality, assume that $\delta_0(t)=0$. Let $\tilde{\theta}_k(t)=M_k\tilde{\delta}_k(t)$, then $0=\sum_{k=1}^{n}\tilde{\theta}_k(t)$. The condition $d\tilde{\theta}_k(t)/dt=0$ defines the equilibrium rotor angles $\tilde{\theta}_k{}^s$ in terms of $P_{mk}-E_k{}^2G_{kk}$. Introducing $\theta_k(\ )=\tilde{\theta}_k(t)-\tilde{\theta}_k{}^s$ and linearizing about $\theta_k(t)=0$, we have

$$\frac{d^2\theta_k(t)}{dt^2}+2a_k\frac{d\theta_k(t)}{dt}+\tilde{\omega}^2\theta_k(t)=\sum_{j=1}^{n}c_{jk}\theta_j(t) \quad (1.2)$$

where $\tilde{\omega}_k{}^2=\sum_{j=1}^{n}E_kE_jB_{kj}/M_k$, $a_k=\frac{1}{2}d_k/M_k$, and $c_{kj}=E_kE_jB_{kj}/M_j$ defines the coupling. Defining the average coupling $\bar{c}_k=(\sum_{j=1}^{n}c_{kj})/n$, and $c_{kj}=\bar{c}_k+\Delta c_{kj}$, we assume that

(A1) $\Delta c_{kj}(t)=\varepsilon\mu_{kj}(t)$

where $\varepsilon>0$ is a parameter and $\mu_{kj}(t)$ are zero mean, ergodic Markov processes. In this notation (1.2) becomes

$$\frac{d^2\theta_k{}^\varepsilon(t)}{dt}+2a_k\frac{d\theta_k{}^\varepsilon(t)}{dt}+\tilde{\omega}_k{}^2\theta_k{}^\varepsilon(t)=\varepsilon\sum_{j=1}^{n}\mu_{kj}(t)\theta_j{}^\varepsilon(t) \quad (1.3)$$

$$\theta_k{}^\varepsilon(0), d\theta_k{}^\varepsilon(0)/dt \text{ given, } k=1,2,\ldots,n.$$

The assumption (A1) says that the incremental coupling $\Delta c_{kj}(\cdot)$ is "weak", i.e., of order ε, a small parameter, fluctuating with zero average value. The fluctuations may be regarded as due to small, random variations in the load impedances or variations in the transmission line reactances. Operating power systems are always subject to fluctuations of this type. We assume also that

(A2) $\alpha_1=0$; $0<\alpha_2<\ldots<\alpha_n$; $\tilde{\omega}_k>\alpha_k$; $k=1,2,\ldots,n$.

That is, the first machine has zero net damping, a realistic situation [1], and the other machines are dissipative.

Theorem 1.1: If (A1)-(A2) hold, then there is an $\varepsilon_0>0$ such that for ε fixed $0<\varepsilon\leqq\varepsilon_0$, we have

$$\lim_{t\to\infty}[(\theta_1{}^\varepsilon(t))^2+(\dot{\theta}_1{}^\varepsilon(t))^2]^{\frac{1}{2}}=\infty \quad (1.4)$$

almost surely, provided that

$$b\equiv\sum_{k=2}^{n}\frac{1}{2\omega_1\omega_k}\int_0^\infty e^{-a_kt}E[\mu_{1k}(t)\mu_{k1}(0)]\sin\omega_1t\sin\omega_kt\,dt < \frac{1}{4\omega_1{}^2}\int_0^\infty E[\mu_{11}(t)\mu_{11}(0)]\cos\alpha\ \omega_1t\,dt\equiv a \quad (1.5)$$

where $\omega_k=(\tilde{\omega}_k{}^2=\alpha_k{}^2)^{\frac{1}{2}}$.

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The asymptotic growth rate in (1.4) is exp $[(a-b)\varepsilon^2 t]$. The self coupling effect a is positive and destabilizing. The cross coupling effect b can have either sign and may induce either stability or instability. Notice that only the second order statistics of $\mu_{kj}(t)$ enter in the expression (1.5). That small, random, zero mean, coupling between a strongly dissipative system and a marginally stable system can induce a gross instability in the latter is somewhat surprising.

This result was first proved in a general setting by Papanicolaou and Kohler [2], except for some details settled by the methods of [3]. It was applied to the power system dynamic instability problem in [4][5].

As Papanicolaou and Kohler note [2], this system and its analysis belong to a class of problems involving generalized master equations as their descriptive base. Master equations have been used in mathematical physics to study the time evolution of open quantum mechanical systems, providing, for example, a framework for the study of irreversibility. We shall review the salient points of this theory in the next section. The primary concern of the theory is the analysis of the dynamic evolution of a study system S moving (irreversibly) under the influence of its surroundings B. In the parlance of control theory the overall system $S \oplus B$ is a large scale system with S the local subsystem of interest and B the remaining system which is usually represented by an "equivalent." The obvious subdivision of the coupled oscillator system (1.1) is typical.

In general, a complete analysis of the "open" system S requires a microscopic description of the total "closed" system $S \oplus B$. By eliminating the coordinates of B from the latter one can infer the behavior of S. Systems which may be treated in this way include the damped harmonic oscillator as a paradigm for more complex systems (e.g., spin systems), or lasers in which S is the radiation output and B includes the pump, loss mechanisms, and active atoms [6]. The mathematical description of these systems takes its most coherent form in the use of "master equations" to capture the time evolution of (probability) distributions for the variables of interest. These equations, as we shall see, typically contain memory effects. They are most useful in (Markovian) cases when these effects may be neglected ([6], p. 101). Our treatment focusses on the form of the master equation in the asymptotic limit of weak coupling between S and B. We begin with the simple problem of line broadening in a perturbed harmonic oscillator and then consider the analysis of abstract master equations for more complex phenomena.

2. Resonance and Relaxation Phenomena

The analysis of the energy versus frequency spectrum of a physical system is fundamental to obtaining information about the system. The shapes of spectral "lines" can provide rather specific information in certain cases, including the possible internal motion of nuclei in a molecular system in nuclear magnetic resonance (NMR) experiments [7]. A line shape function is simply the (normalized) Fourier transform of the correlation function of a physical variable

$$I(\nu)=\frac{1}{2\pi}\int_{-\infty}^{\infty}\langle x^*(t)x(0)\rangle \exp(-i\nu t)dt/\langle x^*x\rangle. \quad (2.1)$$

In engineering parlance, $I(\nu)$ is the power spectral density function. In (2.1) $\langle\cdot\rangle$ is the ensemble average.

Consider the oscillator

$$\dot{x}(t)=i\Omega(t)x(t) \quad (2.2)$$

where the oscillation frequency $\Omega(t)$ includes random modulation by the environment; that is, $\Omega(t)=\omega_0+\omega(t)$ with $\langle\omega(t)\rangle=0$. (The precession of a spin moment in a magnetic field is described by (2.1) with $\Omega(t)=\gamma H(t)$, $H(t)=H_0+H_1(t)$). In the scalar case we have

$$\langle x(t)x^*(0)\rangle=|x(0)|^2 e^{i\omega_0 t}\phi(t) \quad (2.3)$$

where

$$\phi(t)=\langle\exp\, i\int_0^t \omega(s)ds\rangle \quad (2.4)$$

is the relaxation function. The resonance absorption spectrum (unnormalized) is

$$\tilde{I}(\nu-\omega_0)=\frac{1}{2\pi}\int_{-\infty}^{\infty}e^{-i(\nu-\omega_0)t}\phi(t)dt; \quad (2.5)$$

and it is $\tilde{I}$ which is observed directly. The random modulation $\omega(t)$ effectively broadens $\tilde{I}(\nu-\omega_0)$ about the center frequency ω_0. Physical observations of the absorption of electromagnetic waves by a large number of independent magnetic spins, the ensemble, will correspond to this kind of ensemble averaging.

The parameters

$$\Delta^2=\langle\omega^2(t)\rangle,\ \tau=\int_0^{\infty}\langle\omega(t)\omega(0)\rangle dt/\Delta^2 \quad (2.6)$$

describe the intensity of the interaction and the correlation time of the modulation, respectively. The condition $\Delta\tau>>1$ is slow modulation and $\Delta\tau<<1$ is fast modulation. Roughly, for slow modulation the line shape $I(\nu)$ mimics the probability distribution of Ω. In fast modulation the spectrum shows the effects of motional narrowing - the line shape becomes sharp with a Lorenzian form.

This is illustrated in the case when $\omega(t)$ is Gaussian with $\langle\omega(t)\omega(0)\rangle=\Delta^2\exp(-|t|/\tau)$. Then

$$\phi(t)=\exp[-\Delta^2\tau^2(e^{-t/\tau}-1+t/\tau)] \quad (2.7)$$

$$\tilde{I}(\nu)=\frac{1}{\pi}\mathrm{Re}\int_0^{\infty}\exp[-\Delta^2\tau^2(e^{-t/\tau}-1+t/\tau)-i\nu t]dt.$$

One can show that ([8], p. 30)

$$\tilde{I}(\nu-\omega_0)\cong\begin{cases}\exp[-(\nu-\omega_0)^2/2\Delta^2]\sqrt{2\pi}\Delta, & \Delta\tau>>1\\ \frac{1}{\pi}(\Delta^2\tau)/[(\nu-\omega_0)^2+(\Delta^2\tau)^2], & \Delta\tau<<1\end{cases} \quad (2.8)$$

The second, Lorenzian line shape has width $2\Delta^2\tau$ and it is clear that the line is much narrowed. In NMR studies the thermal motion of nuclei causes this kind of (motional) narrowing.

As a second example consider a two level atom (ground state and excited state with energy level $h\Omega$) subject to random perturbations, i.e., a random electric field $E(t)$ [9]. The Schrödinger equation for the wave vector $\psi=[\psi_1,\psi_0]$ is

$$\frac{d}{dt}\begin{pmatrix}\psi_1\\ \psi_2\end{pmatrix}=\begin{pmatrix}-i\Omega & 0\\ 0 & i\Omega\end{pmatrix}\begin{pmatrix}\psi_1\\ \psi_2\end{pmatrix}-i\alpha E(t)\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}\begin{pmatrix}\psi_1\\ \psi_2\end{pmatrix} \quad (2.9)$$

where $\hbar\alpha$ is the matrix element of the dipole moment between the two states. The stationary random process $E(t)$ is assumed to have $\langle E(t)\rangle=0$, $\langle E^2(t)\rangle=1$, and correlation time τ. The problem is to describe the probability distribution of ψ when $\alpha\tau$ is small.

Consider the simpler problem of analyzing the second moments, i.e., averages of

$$u_1=\psi_1^*\psi_1,\ u_2=\psi_0^*\psi_0,\ u_3=\psi_1^*\psi_0,\ u_4=\psi_0^*\psi_1. \quad (2.10)$$

Set $u=[u_1,\ldots,u_4]^T$. Then

$$\dot{u}(t)=A_0u(t)+i\alpha E(t)\tilde{A}_1u(t) \quad (2.11)$$

where $A_0=\text{diag}\{1,1,i\Omega,-i\Omega\}$ and $\tilde{A}_1=\tilde{A}_1{}^T$ has $a=\begin{bmatrix}-1 & 1\\ 1 & -1\end{bmatrix}$ on the off diagonal blocks and 0_{2x2} on the diagonal. Consider the change of coordinates

$$v(t)=\exp(-A_0t)u(t)$$
$$A_1(t)=\exp(-A_0t)A\ \exp(A_0t). \quad (2.12)$$

Then

$$\frac{dv}{dt}=i\alpha E(t)A_1(t)v(t). \quad (2.13)$$

Since $E(t)$ has zero mean the effects of the coefficients are $O(\alpha^2)$. Using averaging theory for this problem (e.g.[10]), one can show that the mean $\langle v(t)\rangle=\bar{v}(t)$ satisfies to $O(\alpha)$ the averaged equation

$$\frac{d\bar{v}}{dt}=\alpha^2\overline{A_1A_1}\bar{v}(t) \quad (2.14)$$

where

$$\overline{A_1A_1}=\lim_{T\to\infty}\int_0^T\int_0^t\langle E(t)E(s)\rangle A_1(t)A_1{}^*(s)ds\ dt$$
$$=\text{diag}\left\{\begin{bmatrix}-a & a\\ a & -a\end{bmatrix};\begin{bmatrix}-a+ib\\ a-ib\end{bmatrix};\begin{bmatrix}a+ib\\ -a-ib\end{bmatrix}\right\} \quad (2.15)$$

with

$$\tfrac{1}{2}(a+ib)=\int_0^\infty\langle E(t)E(t-s)\rangle e^{i\Omega s}ds. \quad (2.16)$$

It follows that the mean of $u(t)$, say $\bar{u}(t)$, satisfies (to $O(\alpha)$)

$$\frac{d\bar{u}(t)}{dt}=(A_0+\alpha^2\overline{A_1A_1})\bar{u}(t) \quad (2.17)$$

The coefficient matrix has one zero eigenvalue which corresponds to an equilibrium state $|\psi_1|^2=|\psi_0|^2=1/2$ in which both states are occupied with the same probability, rather than with the Boltzmann distribution. This flaw is inherent in (2.9) in which the perturbing field $E(t)$ causes state transitions in either direction with equal probability.

The model

$$\frac{dM}{dt}=\gamma[H(t)+H_0]\ X\ M(t) \quad (2.18)$$

for a spin moment $M(t)$ in a magnetic field (H_0= steady external field, $H(t)$=stochastic magnetic field describing the surrounding lattice) suffers the same defect; specifically, under natural assumptions on $H(t)$ the spin relaxes to zero instead of to the equilibrium corresponding to the external field [11]. In [11] Kubo and Hashitsume modified (2.18) by introducing a frictional term, not unlike the frictional force in the Langevin theory of Brownian motion, obtaining

$$\frac{dM}{dt}=\gamma[H_0+H(t)]\ X\ M(t)-\kappa[H_0\ X\ M(t)]\ X\ M(t) \quad (2.19)$$

By a formal argument they were able to show that $M(t)$ relaxes to χH_0 for certain values of κ. The latter is chosen by invoking the "fluctuation - dissipation" theorem (*)[12] to balance the intensity of the fluctuations $H(t)$ and the dissipation to maintain the proper temperature. A phenomenological treatment of this type is possible for the two-state model (2.9); however, this kind of analysis is somewhat arbitrary and unsatisfying, especially when nonlinear models like (2.19) are required.

These formulations provide an incomplete description of the interaction between the system and its surroundings, particularly the influence of the former on the latter. In the Kubo paradigm the force produced by the surroundings acting upon the system behaves like a Gaussian process. In order to validate this model one should take steps similar to those in the proof of the central limit theorem, deriving the cumulative force from an interaction Hamiltonian composed of a large number of terms. This point was recognized in the formal treatments of "master equations" in [13][14](among others); however, the lack of a precise analysis and range of validity of the conclusions makes this work less compelling than it might otherwise be.

3. Markovian Master Equations

In [15]-[17] E.B. Davies gives a careful treatment of master equations in the asymptotic limit of weak coupling in which the system response becomes Markovian. In this (generalized) diffusion limit the important conclusions regarding resonance and relaxation behavior states earlier can be rigorously defended. What follows is a brief sketch of Davies's treatment of the Nakajima-Zwanzig master equation [6].

Consider a closed system $S\oplus B$ consisting of two interacting parts S and B. The state of $S\oplus B$ is defined by the density operator $V(t)$ which satisfies the Liouville-von Neumann equation

$$V(t)=-(i/h)[H,V(t)]=-LV(t). \quad (3.1)$$

(*) This result is perhaps best known to electrical engineers in the form of the Nyquist theorem for the thermal noise in an impedance. Nyquist showed that the random electromotive force appearing across a resistor is determined by its impedance. See his 1928 paper in Physical Review, vol. 32, or [12].

The Hamiltonian H is time-invariant since the system $S \oplus B$ is closed. It, and so L, consists of three parts

$$H=H_S+H_B+H_{SB}$$
$$L=L_S+L_B+L_{SB} \qquad (3.2)$$

corresponding to the free motion of S and B (each is a system in its own right) and an interaction, respectively. The free motion of S and B ($L_{SB}=0$) is described by a one parameter group U(t) on some Banach space X. Assuming the U(t) is strongly continuous, its infinitesimal generator $L=L_S+L_B$ is closed and densely defined. Let P_0 be a projection so that $P_0X=X_0$ is the state space S and $P_1X=(1-P_0)X=X_1$ that of the bath. Evidently, U(t) leaves both X_0 and X_1 invariant. We have $L_S=P_0\tilde{L}$, $L_B=P_1\tilde{L}$ with $[P_0,\tilde{L}]=0$, etc.

The interaction L_{SB} represents a perturbation which is assumed to be bounded operator εA on X. Writing $A_{ij}=P_iAP_j$, we assume $A_{00}=0$ for simplicity. Then $L_{SB}=(A_{01}+A_{10}+A_{11})$. The parameter $\varepsilon>0$ is introduced to monitor the intensity of tne interaction. Let $U^\varepsilon(t)$ be the group generated by $\tilde{L}+\varepsilon A_{11}$ so that $[U^\varepsilon(t), P_0]=0$ for all t. The total system is described by $V(t)=V^\varepsilon(t)$ from (3.1) which satisfies

$$V^\varepsilon(t)=U^\varepsilon(t)+\varepsilon\int_0^t U^\varepsilon(t-s)(A_{10}+A_{01})V^\varepsilon(s)ds. \qquad (3.3)$$

To obtain the master equation for the description of S, we use the projections

$$P_0V^\varepsilon(t)P_0=U^\varepsilon(t)P_0+\varepsilon\int_0^t U^\varepsilon(t-s)A_{01}P_1V^\varepsilon(s)P_0ds$$
$$P_1V^\varepsilon(t)P_0=\varepsilon\int_0^t U^\varepsilon(t-s)A_{10}P_0V^\varepsilon(s)P_0ds. \qquad (3.4)$$

Defining $W^\varepsilon(t)=P_0V^\varepsilon(t)P_0$, the density (operator) of S, we have (in X_0)

$$W^\varepsilon(t)=U(t)+\varepsilon^2\int_0^t\int_0^s U(t-s)A_{01}U^\varepsilon(s-r)A_{10}W^\varepsilon(r)dr\, ds \qquad (3.5)$$

where $U^\varepsilon(t)P_0=U(t)$ because $A_{00}=0$.

This is the integrated form of the master equation. To obtain the differential form, set $\zeta^\varepsilon(t)=W^\varepsilon(t)\zeta$, $\zeta\epsilon X_0$. Then formally

$$\frac{d\zeta^\varepsilon}{dt}=-iL_S\zeta^\varepsilon+\varepsilon^2\int_0^t A_{01}U^\varepsilon(t-s)A_{10}\zeta(s)ds \qquad (3.6)$$

and this is the master equation in the form developed by Nakajima and Zwanzig. The memory effect is evident.

As a description of a large category of phenomena (see [6]), the master equation is an extremely flexible concept. However, as Haake points out, there are limits to its practical (computational) usefulness. Unless the memory effects can be neglected in some systematic way, usually by exploiting expansions in terms of small parameters, the generalized master equation (3.6) is an "empty concept"[6], p. 101.

In [15]-[17] Davies studies the weak coupling limit ($\varepsilon\to0$) in which the asymptotic form of the master equation becomes, after rescaling, memoryless or Markovian. The setup is as follows: let $\tau=\varepsilon^2t$ be the slow time scale and $Y^\varepsilon(\tau)=U(-\tau/\varepsilon^2)W^\varepsilon(\tau/\varepsilon^2)$ the interaction coordinates (recall (2.12)-(2.14)). Then

$$Y^\varepsilon(\tau)=1+\int_0^\tau H^\varepsilon(\tau-\sigma,\sigma)Y^\varepsilon(\sigma)d\sigma \qquad (3.7)$$

when

$$H^\varepsilon(\tau,\sigma)=U(-\sigma/\varepsilon^2)K^\varepsilon(\tau)U(\sigma/\varepsilon^2)$$
$$K^\varepsilon(\tau)=\int_0^{\tau/\varepsilon^2}U(-s)A_{01}U^\varepsilon(s)A_{10}ds. \qquad (3.8)$$

Restricting attention to the case X_0 finite dimensional (this is removed in [16], Davies's limit theorem is:

Theorem 3.1: ([15], Theorem 2.1). Suppose for all $\tau_1\geq0$, $\exists c$ such that $||K^\varepsilon(\tau)||\leq c$ for $|\varepsilon|\leq1$, $0\leq\tau\leq\tau_1$. Suppose also $\exists K$: $X_0\to X_0$, bounded, such that if $0<\tau_0<\infty$, then $\lim_{\varepsilon\to0}||K^\varepsilon(\tau)-K||=0$ uniformly in τ, $\tau_0\leq\tau\leq\tau_1$. Then for $x\epsilon X_0$

$$\lim_{\varepsilon\to}||Y^\varepsilon(\tau)x-Y(\tau)x||=0 \qquad (3.9)$$

uniformly in $0\leq\tau\leq\tau_1$, where

$$Y(\tau)=\exp(\overline{K}\tau),\overline{K}=\lim_{\to\infty}\frac{1}{2T}\int U(s)KU(-s)ds \qquad (3.10)$$

and $\overline{K}U(t)=U(t)\overline{K}$ as operators on X_0 for all t.

Remarks: 1. If $A_{11}=0$ (and $A_{00}=0$), then $U^\varepsilon(t)=U(t)$ and one can take

$$K=\int_0^\infty U(-s)A_{01}U(s)A_{10}ds. \qquad (3.11)$$

The case $A_{11}\neq0$ is more complex, see [6], Theorem 2.3.

2. The limiting evolution of S in the slow time is $dY(\tau)/d\tau=\overline{K}Y(\tau)$, a quantum - mechanical Fokker - Planck equation (see the example in [15]). The original model (3.1) on X is fully reversible; however, the limit (3.9) leads to a semigroup on X which represents an irreversible dissipative process. The origin of irreversibility is inherent in the weak coupling limit.

3. The formal similarity of this limit theorem and those for stochastic differential equations on a Banach space X_0 may be demonstrated by setting $X=L^1(\Omega,X_0,P(d\omega))$, where (Ω,P) is the sample space, and $P_0f=\int_\Omega f(\omega)P(d\omega)$. The interaction is $(L_{SB}f)(\omega)=A(\omega)f(\omega)$, where A is a random operator. See [17] [18] for a more complete discussion of this point.

4. In [19] J. Pulé adapts Davies's model to derive the phenomenological Bloch equations for time evolution of a spinor interacting with a heat bath of harmonic oscillators in equilibrium. Since the particle is different from those constituting the bath, some modifications are necessary. The analysis centers on the weak coupling limit, and it employs the rescaling of time and the transformation to the interaction picture. Despite its complexity, the treatment is natural, within its limits, and more satisfying than the ad hoc adoption of

phenomenological terms.

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