A Pair of Interacting Spins Coupled to an Environmental Sea: Dissipation and Mutual Coherence

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We consider the quantum dynamics of two spin-1/2 systems, each coupled to a bath of oscillators, so that a bath-mediated coupling is generated between the spins. We find that the interaction destroys any coherent motion of the 2 spins, even if the coupling of each spin to the bath is quite weak, unless the interaction is extremely small. This is because the dynamic mutual bias between the spins blocks any coherent transitions between nearby degenerate states. In many quantum measurement operations this means that decoherence effects will be much stronger during the actual measurement.

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In this paper we study the theoretical problem of a Pair of Interacting Spins Coupled to an Environmental Sea (we use the acronym “P.I.S.C.E.S.” for brevity). The 2 spins will each be described as 2-level systems, and we shall concentrate on environments that can be represented as a spin bath [3,4]. Our PISCES model is clearly a generalisation of previous models like the “spin-boson” model, describing a single spin coupled to a sea of oscillators - this model has been widely studied in connection with the Kondo problem [8], quantum diffusion [6], SQUID tunneling [2], and magnetic grains [10], and extensively reviewed (see, eg., refs. [11]).

The interest of the PISCES model is in the way it reveals a dual role of the environment - whilst it causes decoherence and dissipation in the motion of each spin, one also expects that it might cause some mutual coherence between them. For very weak mutual coupling (as in the problem of two 2-level atoms coupled radiatively) this mutual coherence is fairly well understood. However, as we shall see, a radical change occurs once the coupling exceeds a very small value, to be specified below. One then finds quantum relaxation behaviour of the 2 spins, even at temperature $T = 0$. Since the majority of PISCES problems, in condensed matter and elsewhere, have couplings exceeding this value, our results have important practical application. The PISCES model is also a primitive model for quantum measurements, in which both dissipation and the back-reaction of the measuring apparatus on the measured system are included.

In cases where the environment is modelled by an oscillator bath, we will start from an effective Hamiltonian $H_{PISCES} = H_0 + H_{\text{int}}$, between spins located at position $\mathbf{r}_1$ and $\mathbf{r}_2$, where

$$H_0 = -\frac{\hbar}{2} (\Delta_1 \tau_1^x + \Delta_2 \tau_2^x) + \frac{1}{2} \sum_k m_k (x_k^2 + \omega_k^2 z_k^2)$$  \hspace{1cm} (1)$$

$$H_{\text{int}} = \frac{1}{2} K_{\alpha \beta} \tau_1^\alpha \tau_2^\beta$$

$$+ \frac{1}{2} \sum_k (q_{01} c_k^{(1)} e^{i k \cdot \mathbf{r}_1} \tau_1^x + q_{02} c_k^{(2)} e^{i k \cdot \mathbf{r}_2} \tau_2^-) x_k$$ \hspace{1cm} (2)$$

where $\tau_j^\alpha$ are the Pauli operators for each spin ($j = 1,2$), and $\{x_k\}$ are the bath oscillators. In this paper we are really interested in the indirect bath-mediated interaction between $\tau_1$ and $\tau_2$, but we include also a direct interaction $K_{\alpha \beta}(\mathbf{r})$, with $\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2$. $K_{\alpha \beta}(\mathbf{r})$ can be considered as modelling the static part of some other field-mediated interaction [1]. We assume that $k$ is a momentum index, describing delocalised bath modes; we also ignore non-diagonal couplings (ie., couplings in $\tau_j^x$ or $\tau_j^y$), which have a less important effect on the physics [6,9]. Clearly our model could be generalised, but at the expense of great complexity, and we believe that [8] and [9] bring out most of the essential physics.

The interactions with the bath are characterised by spectral functions $J_j(\mathbf{r}, \omega)$ whose diagonal elements $J_j(\omega) \equiv J_{jj}(\omega)$, referring to self-interactions of $\tau_j$ via the bath, have the Caldeira-Leggett form [2]:

$$J_j(\omega) = \frac{\pi}{2} \sum_k \frac{|c_k^{(j)}|^2}{m_k \omega_k} \delta(\omega - \omega_k)$$ \hspace{1cm} (3)$$

The off-diagonal elements have a complicated form if $|\mathbf{r}|$ is large, because of retardation effects [12]; these begin to be important once $\omega_k \geq v_k / |\mathbf{r}|$, where $v_k$ is the velocity of propagation of the $k\text{th}$ oscillator mode. Here, we shall ignore such effects (but see ref. [13]) which are most important in the weak-coupling limit, so that

$$J_{12}(\mathbf{r}, \omega) = \frac{\pi}{2} \sum_k \left| c_k^{(1)} D_k(0) c_k^{(2)*} e^{i k \cdot \mathbf{r}} \right| \frac{1}{m_k \omega_k} \delta(\omega - \omega_k)$$ \hspace{1cm} (4)$$

where $D_k(0)$ is the static limit of the oscillator bath propagator [12].

We shall consider two forms [14] for $J_{jj}(\mathbf{r}, \omega)$. The Ohmic form $J_{jj}(\mathbf{r}, \omega) = \omega \eta_j e^{-|\mathbf{r}|/\delta \eta_j}$, with $\eta_j \equiv \eta_{jj}$ a local friction coefficient and $\delta \eta_2 \sim (\eta_1 \eta_2)^{1/2} \nabla e(\mathbf{r})$, is
appropriate to eg., electrons in Fermi liquid. The superionic $J_{ij}(r, \omega) = \tilde{g}_{ij}(r) \Theta_B(\omega / \Theta_T)m e^{-\omega / \Theta_T}$ applies to phonons or photons, with $m \geq 3$ in 3 dimensions [2]; now $\tilde{g}_{12} \sim (\tilde{g}_{1} \tilde{g}_{2})^{1/2} \Phi_\omega(r)$. For electrons $|V_{\phi}(r)| \sim \cos(2kFR)/(kFR)^3$ (the RKKY form) in 3 dimensions; for phonons $|V_{\phi}(r)| \sim (ao/\theta)^3$, where $ao$ is the lattice spacing. The values of the upper cut-offs $\Omega_0$ and $\Theta_D$ are typically $\Omega_0 \sim eV'$ for electrons, and $\Theta_D \sim 10^{-2}eV$ for phonons.

We also define a mutual bias function $\tilde{e}(r)$ as

$$\tilde{e}(r) = \frac{-q_{01}q_{02}}{\pi} \int_0^\infty \frac{d\omega}{\omega} J_{12}(r, \omega)$$

with sign such that positive/negative $\tilde{e}(r)$ corresponds to ferromagnetic/antiferromagnetic coupling between $\tau_1$ and $\tau_2$. Defining $\alpha_{ij}(r) = \eta_{ij}(r)\eta_{0i}\eta_{0j}/2\pi\hbar$, one then has

$$\tilde{e}(r) = \begin{cases} 
-2\hbar \Omega_0 \alpha_{12}(r) & \text{(Ohmic)} \\
-2\hbar \Gamma(m) \Theta_D \tilde{g}_{12}(r) & \text{(Superohmic)}
\end{cases}$$

with $\tilde{e}$ proportional to the upper cut-off frequency in both cases [3].

A complete study of this problem calculates the 16 elements of the 2-spin density matrix $\rho(\tau_1, \tau_2, t; \tau'_1, \tau'_2, t')$. To do this we use standard influence functional techniques [3]: the total influence functional $F\{\tau_1, \tau_2\}$ can be factored as $F = F_{11} F_{22} F_{12}$, where $F_{11}$ and $F_{22}$ are identical to the single spin-boson functionals, and $F_{12}$ contains all dynamic couplings via the bath. $F_{12}$ is a functional over the paths of both spins together, and is thus intrinsically more complex than $F_{11}$ and $F_{22}$; it cannot be evaluated in closed form for arbitrary values of the parameter $\omega$ in (6). The “dilute-blip” approximation [2] cannot be applied to $F_{12}$ in the very weak coupling limit because then it may have overlap in time between arbitrary configurations of each spin - thus this limit must be handled perturbatively [3]. Away from this limit, the mutual bias $\tilde{e}(r)$ plays an essential role. As a function of time the coupling energy in a path integral contribution to $\tilde{\rho}(t)$ flips between $\pm \tilde{e}(r)$; once $|\tilde{e}(r)|$ is large enough its effect is to suppress configurations in which both spins are simultaneously in blip states. One may then use a dilute-blip approximation for $F_{12}$. The parameter regime in which this works depends on the precise form of $J_{ij}(r, \omega)$; we give the limits of validity below, for the ohmic and superohmic cases [3].

There is no space here to give results for all matrix elements of $\tilde{\rho}$ (see ref. [3]); here we concentrate on $P_{++}(t)$, the probability to find the system in the state $| \uparrow \uparrow \rangle$ at time $t$, if at $t = 0$ it was also in state $| \uparrow \uparrow \rangle$. Then for ferromagnetic coupling ($\alpha_{12} > 0$) we find

$$P_{++}(t) = A_+ + A_+ e^{-(\Gamma_1 + \Gamma_2)t} + B_+ e^{-R_1 t} + B_- e^{-R_2 t}$$

$$A_+ = \frac{1}{4} [1 \pm \tanh(\bar{e}/2kT)]$$

with the functions $\Gamma(x)$ on the right-hand side being Gamma functions. If there were no interactions at all between $\tau_1$ and $\tau_2$, then at $T = 0$, the $\tau_i$ would freeze for $\alpha_j > 1$, relax exponentially (with power law corrections) for $1/2 < \alpha_j < 1$, and show damped oscillations for $\alpha < 1/2$; at any finite $T$, the $\tau_i$ would relax exponentially for any value of the $\alpha_j$ (see ref. [4]).

Switching on the interaction $J_{12}(r, \omega)$ quickly changes this. Suppose, as above, that $\alpha_{12}(r)$ is positive (ferromagnetic). Then once $\tilde{e} \gg kT$, ie., once $\tilde{g}_{12} \gg kT/\Omega_0$, so that $\tanh(\bar{e}/2kT) \sim -1$, then $P_{++}(t) = 1$ for all times of interest, ie., the 2 spins freeze each other! More generally we see that at long times $P_{++}(t)$ relaxes to $\frac{1}{2}[1 + \tanh(\alpha_{12} \Omega_0/kT)]$. A similar freezing to the antiferromagnetic $| \uparrow \downarrow \rangle$ occurs if $-\alpha_{12} \gg kT/\Omega_0$. Since $\Omega_0$ is usually large, this freezing can happen for very small coupling at low $T$. The results are valid if $\Delta_j \ll |\alpha_{12}| \Omega_0$, at any $T$, or for any $\alpha_{12}$ if $kT \gg \Delta_j/\alpha_j$. In cases where the $\Delta_j$ describe tunneling matrix elements, as in SQUID’s, quantum diffusion [2], or magnetic grains [3], the tunneling rates are often rather small and so the results apply for very small couplings $\alpha_{12}$; the same will be true for many metallic glasses.
Similar results are obtained in the superohmic case, for which
\[ \Gamma_j = (g_{0j} \Delta_j / \epsilon)^2 J_j(\epsilon) \coth(\epsilon/kT) \]  
(16)
In the common case where \( m = 3 \), this gives \( \Gamma_j \sim g_{0j}^2 \Delta_j^2 / \Theta_D \). If \( |g_{12}| \Theta_D \gg kT \), the spins will again be frozen; otherwise we get relaxation according to \( \Delta_j \ll |g_{12}| \Theta_D \), for any \( T \), or for any \( g_{12} \) if \( kT \gg \Delta_j / \Theta_D \). Typically, \( \Delta_j \ll \Theta_D \) and this relaxation will be rather slow. This result shows that the bias \( \epsilon \) plays a crucial role - if there were no coupling between the spins, then they would not freeze even at \( T = 0 \), no matter how large the couplings \( \bar{g}_1 \) and \( \bar{g}_2 \).

Some qualitative features of the results deserve special mention; in particular

(i) It is quite common in phenomenological studies of this problem to simulate the environmental effects on the 2 coupled spins by stochastic terms \([g_5] \). In general such methods will give results quite unlike these (often with oscillatory behaviour in \( \hat{J}(\epsilon) \) for large inter-spin couplings. The reason for the discrepancy is fundamentally that quantum influence functionals cannot be modeled by classical (c-number) noise source \([g_5] \).

(ii) The 3 relaxation times appearing in \( \hat{\rho}(t) \) (see Eq. \([g_5] \)) can be quite different, and their contributions will in general appear in different proportions in the 16 different elements of \( \hat{\rho}(t) \). Fig. \([g_5] \) illustrates this by plotting 4 of these matrix elements (including \( P_{+\pm}(t) \)) calculated in the same way as \([g_5] \).

![FIG. 1. Probabilities of occupation for a system with parameters \( \Gamma_1 = 0.5 \) sec\(^{-1} \), \( \Gamma_2 = 0.7 \) sec\(^{-2} \) and \( \epsilon/2kT = -0.5 \). The system starts at \( t = 0 \) in the state \( |\uparrow\uparrow\rangle \); \( \bar{P}_{\alpha\beta} \) is then the probability that at time \( t \) the system has \( \tau_1^\alpha = \alpha \) and \( \tau_2^\beta = \beta \).](image)

(iii) There is no trace left in our results of the “phase-transition” occuring at \( \alpha = 1/2 \) and \( \alpha = 1 \) in the spin-boson problem at \( T = 0 \), for the case of ohmic dissipation \([g_5] \). The localisation transition at \( \alpha = 1 \) is replaced here by a crossover to localised behaviour, at \( T = 0 \), as \( |\epsilon(r)\rangle = 2\Omega_0 \alpha_{12}(r) \) becomes greater than the larger of \( \Delta_1 \) and \( \Delta_2 \). We can understand this physically as “degeneracy blocking”, i.e., the mutual bias blocks tunneling by destroying the degeneracy between the initial and final states. There is also a finite temperature crossover to localisation, for a finite coupling \( \epsilon(r) \gg \Delta_j \), as one lowers \( T \); this occurs for \( kT \sim 2\Omega_0 \alpha_{12}(r) \), for ferromagnetic coupling, and \( kT \sim -2\Omega_0 \alpha_{12}(r) \), for antiferromagnetic coupling. Analogous crossovers will also exist for superohmic coupling.

A surprising feature of the results (at least for us) is that our solution \([g_5] \) does not allow any mutually coherent oscillations of the two spins. Thus, e.g., in the ohmic problem, if \( \alpha_1, \alpha_2 < 1/2 \), so each spin exhibits damped oscillations if \( \alpha_{12} = 0 \), one might have expected to find that if \( \Delta_1 \sim \Delta_2 \), switching on \( \alpha_{12} \) could cause some kind of “frequency locking” between the 2 spins. Instead one simply finds that the mutual bias destroys the oscillations, once we are out of the very weak perturbative limit. A corollary of this is that if we start off with the 2 coupled spins and no bath, then the effect of coupling in the bath is to destroy coherent oscillations of each spin far more quickly than one would expect from the known destructive effects of the bath on single spin coherence \([g_5] \).

We have no space to discuss detailed applications of these results to particular systems (particularly as \( J_{12}(r, \omega) \) is often long range in \( r \), so that for a system containing many 2-level systems, it is not sufficient to simply examine the 2-spin correlation functions). However our main result, that the coherence-destroying role of the bath is greatly exaggerated once mutual coupling between 2 (or more) systems is allowed, seems to be of general relevance. In particular it shows that during a quantum measurement, decoherence effects will be much stronger during the measurement operation. Consider, e.g., a SQUID exhibiting damped coherent oscillations \([g_5] \) for \( \alpha < 1/2 \). It is clear that when this SQUID is coupled to a measuring apparatus (e.g., another SQUID \([g_5] \), modelled also as a damped oscillatory 2-level system), the coherence will be destroyed unless the mutual coupling \( \alpha_{12} \) is extremely small, i.e., coherence will only persist whilst system and the apparatus are decoupled. A detailed analysis of this example \([g_5] \) takes account of the coupling of each SQUID to the same set of EM field modes (whose detailed form will depend on sample geometry). The inductive part of the interaction which is responsible for the measurement is generated, as in the theory of this paper, by this coupling to the EM bath. One must also account for the resistive coupling of each SQUID’s flux coordinate to separate quasiparticle baths.

Finally we note that application of our results to many real systems will be complicated by the effects of the “spin-bath” of nuclear spins and paramagnetic impurities \([g_5] \), since these spins (a) add a further bias field acting on \( \tau_1 \) and \( \tau_2 \), and (b) can be flipped by a transition of \( \tau_2 \) or \( \tau_2 \), thereby causing further decoherence. The bias
field depends on the polarisation of the nuclear spins, and is particularly important if the system is magnetic. However it can even play a role in SQUID’s, because although the SQUID flux couples only very weakly to the nuclear spins, it couples to a lot of them, and the total energy can easily exceed $\Delta_j$ by several orders of magnitudes.

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[11] The distinction between direct and indirect interactions is partly a matter of theoretical choice - one can change $K_{\alpha\beta}(r)$ (here, $K_{12}(r)$) by adding to it a contribution from the high-energy parts of $J_{12}(r,\omega)$, in the approximation where retardation is ignored. This then lowers the upper cut-off frequency appearing in $J_{12}(r,\omega)$ and implicit in $\bar{\epsilon}(r)$.
[12] Retardation effects will be more important for phonons than for electrons at low T, since $\Theta_D \ll \Omega_0$. We emphasize here that our formalism is not altered by retardation (we simply replace $D_k(0)$ in (4) by the full propagator $D_k(\omega)$), but $J_{12}(r,\omega)$ can no longer be factorised in general, so the results are more complex - see ref. 13 for details.
[13] M. Dubé, M.Sc. thesis (UBC, October 1993), and longer papers in preparation, give a more extensive discussion of our results.
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