DECOHERENCE IN THE SPIN BATH

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We develop a mathematical description of the decoherence caused by "spin baths", such as nuclear spins or magnetic impurities. In contrast to the usual oscillator bath models of quantum environments, decoherence in the spin bath can occur without any dissipation. Given the almost ubiquitous presence of nuclear spins in nature, our results have important consequences for quantum measurement theory, particularly as the decoherence mechanisms in spin baths work very differently from those in oscillator baths.

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A popular argument in quantum measurement theory claims that quantum interference between "macroscopically distinguishable states" of a macroscopic collective coordinate will be rendered unobservable "for all practical purposes" ("F.A.P.P."; see ref. [3]) by interactions with the surrounding environment. Formal treatments of this "environmental decoherence" describe the environment as an oscillator bath, with coordinates $\{x_k\}$ each coupled to the macroscopic coordinate $x$. Thus, e.g., in the symmetric "spin-boson" model a spin-1/2 coordinate will be rendered unobservable "for all practically distinguishable states" of a macroscopic coordinate (for our problem, $\Omega_0$) by interactions with the environment, requiring that the system-environment couplings $V_k$ (such as the $c_k$ in (1)) are small enough so that 2nd-order perturbation theory (in the $V_k$) is accurate.

(a) Oscillator bath models, to be valid for given environment, require that the system-environment couplings $V_k$ such as (1) and (2) have a severe effect on the macroscopic coordinate, the environment oscillators are not modified or determined by this coordinate in an essential way. However the typical couplings to the spin bath ($\alpha_k$, $\xi_k$, and particularly $\omega_k$) are independent of $N$, and not necessarily small.

(b) Spin baths have a very destructive decohering effect; moreover, unlike oscillator baths, there is no particular connection between decoherence and dissipation for such baths, and one often has strong decoherence without any dissipation whatsoever.

(i) Derivation of $H_{\text{spin}}$: The derivation of effective Hamiltonians $H_{\text{eff}}$ like (1) and (2) has been given in detail, for particular examples, for both oscillator baths and spin baths. One first incorporates the "fast" high-frequency bath and system dynamics into a low-frequency "effective action" describing the transitions between the low-energy states of both the bath (truncated, for the spin bath, to the spin-1/2 variables $\{\hat{\sigma}_k\}$ and the system (truncated to 2 levels). From these transition matrix elements, plus any residual interactions, one constructs $H_{\text{eff}}$. The high frequency scale $\Omega_0$ is defined by the fast dynamics of the macroscopic coordinate (for our problem, $\Omega_0 \sim \tau_B^{-1}$, where $\tau_B$ is the "bounce time" required for tunneling transitions between $|\uparrow\rangle$ and $|\downarrow\rangle$). Without the bath, the
system transition proceeds via the "instanton operator" \( K_\pm = \frac{1}{2} \Delta_0 \hat{\tau}_\pm \equiv \frac{1}{2} \hat{\tau}_0 e^{-S_0} \), where \( S_0 \) is the bare tunneling action; this gives \( H_{eff}^t = \frac{1}{2} \Delta_0 \hat{\tau}_x \). Coupling to the spin bath converts this to

\[
K_\pm = \frac{1}{2} \Delta_0 \hat{\tau}_\pm e \sum_{k=1}^{N} \left[ (\delta_k \pm i \phi_k) + (\xi_k \vec{\alpha}_k \pm i \omega_k \vec{\alpha}_k) \hat{\tau}_k \right],
\]

in which (a) \( \delta_k \) describes the adiabatic renormalization of \( S_0 \), due to very high frequency (\( \gg \Omega_0 \)) fluctuations of environmental spins, (b) \( \xi_k \vec{\alpha}_k \cdot \hat{\tau}_k \) describes the effect of fluctuations at frequencies \( \lesssim \Omega_0 \); and (c) the term \( i(\delta_k + \alpha_k \vec{\alpha}_k) \cdot \hat{\tau}_k \) parametrizes the change in the macroscopic spin wave-function \( | \chi_k \rangle \), induced by the macroscopic instanton - defining \( | \chi_{k}^{final} \rangle = \hat{T}_k^{\pm} | \chi_{k}^{in} \rangle \) (with \( \pm \) as for \( \hat{\tau}_\pm \)), we have

\[
T_k^{\pm} = e^{i \int \pm d\tau H_k^{(int)}(\tau)} = e^{i(\xi_k \vec{\alpha}_k \cdot \hat{\tau}_k + \phi_k)},
\]

where \( H_k^{(int)}(\tau) \) describes the interaction between \( \hat{\tau}_k \) and the original macroscopic coordinate (before truncation) during the transition. This form for \( K_\pm \) exhausts all relevant terms in the combined system-environment subspace apart from residual interactions existing before and after the transition. If the field \( \gamma_k \) acting on \( \hat{\tau}_k \), due to the macroscopic system, changes from \( \gamma_{k}^{in} \) to \( \gamma_{k}^{final} \) during the transition, we define \( \omega_{k}^{\pm} = (\gamma_{k}^{final} - \gamma_{k}^{in}) \) and \( 2\omega_{k}^{\perp} \hat{m}_{k} = (\gamma_{k}^{final} \pm \gamma_{k}^{in}) \). Adding these couplings then leads directly to (2). The calculation of the various parameters in (2), for both SQUID’s and magnetic grains, starting from microscopic Hamiltonians, has been given elsewhere.\( \square \). Thus, e.g., in the much-studied case of an easy-axis, easy-plane magnetic grain the hyperfine coupling between the "giant spin" \( \vec{S} \) and the nuclear coordinates \( \{ \vec{\alpha}_k \} \) is \( \frac{1}{2} \omega_0 \tau \sum_k \vec{\alpha}_k \) for spin-1/2 nuclei (here \( \vec{S} = S \vec{\tau} \) with \( S \gg 1 \)); this gives \( \omega_{k}^{\perp} = \omega_0 \), \( \omega_{k}^{\parallel} = 0 \), \( \delta_k = \phi_k = 0 \), and, in the usual case where \( \omega_0 \ll \Omega_0 \) (typically \( \omega_0 / \Omega_0 \sim 10^{-2} - 10^{-1} \), one has \( \alpha_k \vec{\alpha}_k = \vec{\alpha}_k \omega_0 / 2\Omega_0 \), and \( \xi_k \vec{\alpha}_k = \vec{\alpha}_k \omega_0 / 2\Omega_0 \) (with \( \vec{\alpha}_k \) - unit vector in the easy-axis direction).\( \square \). All these parameters are clearly independent of the number \( N \) of nuclear spins.

(ii) **Decoherence:** A general analysis of \( \square \) is very lengthy\( \square \). Here we wish to show how decoherence arises, independently of any dissipation. We start by considering a special case of (2), where

\[
\hat{H}_{eff} = -\frac{1}{2} \Delta_0 \hat{\tau}_x e c \sum_{k=1}^{N} \alpha_k \vec{\alpha}_k \cdot \hat{\tau}_k + \frac{1}{2} \hat{\tau}_x \omega_0 \sum_{k=1}^{N} \vec{\alpha}_k \cdot \hat{\tau}_k + H.c.,
\]

so \( \phi_k = \xi_k = \omega_0 = 0 \), and \( \omega_k = \omega_0 \) (\( \delta_k \) is absorbed into a renormalised \( \Delta_0 \)). We also assume \( \omega_0 \gg \Delta_0 \) (typical hyperfine frequencies \( \omega_0 \sim 50 - 5000 \text{ MHz} \), whereas for macroscopic system \( \Delta_0 < 1 \text{ MHz} \); this means that the projection, along the macroscopic coordinate axis \( \hat{\tau}_x \), of the total environmental spin polarization \( \hat{\mathcal{P}} \), remains constant. Any change must involve a minimum energy transfer between system and spin bath, whereas only a maximum of \( \Delta_0 \) is available. Thus no energy is exchanged, and there is no dissipation.

Consider now the diagonal density matrix element \( P(t) = \langle \hat{\tau}_z(t) \hat{\tau}_z(0) \rangle \), i.e., the probability that the macroscopic coordinate is \( | \uparrow \rangle \) at time \( t \) and at time = 0. Without the spin bath \( P(t) = P_0(t) = 1/2[1 + \cos \Delta_0 t] \), and the spectral function \( \chi'(\omega) = i \hat{\mathcal{M}} / d\tau P(t) \exp(-i\omega \tau) \) is \( \chi_0'(\omega) = \pi \delta(\omega - \Delta_0) \), showing perfect coherence. With the spin bath one has

\[
P(t) = \sum_{n=0}^{\infty} \frac{\theta(t)}{2\pi} \int \frac{d\xi}{2\pi} \int \frac{d\xi'}{2\pi} \langle \hat{T}_{2n}[\xi] \hat{T}_{2n}[\xi'] \rangle,
\]

where the sums \( \sum_{nm} \) are over all possible instanton sequences (i.e., "paths"), and

\[
\hat{T}_{2n}[\xi] = \prod_{k=1}^{N} \left[ e^{i\xi_2 \vec{\alpha}_k \cdot \vec{\sigma}_k} e^{-i\alpha_k \vec{\alpha}_k \cdot \vec{\sigma}_k} \cdots e^{i\xi_1 \vec{\alpha}_k \cdot \vec{\sigma}_k} \right],
\]

contains the relevant operator sequences for each path. The "constant polarization" restriction is incorporated via a projection operator

\[
\delta(\hat{\mathcal{P}} - M) = \int \frac{2\pi}{2\pi} \hat{T}_{2n}[\xi] \hat{T}_{2n}[\xi'] \langle \hat{\tau}_z(\hat{\tau}_z - M) \rangle,
\]

inserted into \( \hat{T}_{2n} \); in Eq.(3) we assume the polarization is actually zero. In the usual case where \( \alpha_k \ll 1/N^{1/2} \) (so \( \alpha_k \sim \pi \omega_0 / 2\Omega_0 \)),\( \square \) yields, for polarization = \( M \),

\[
P_M(t) = \int dx e^{-x^2} \left[ 1 + \cos \left( \Delta_0 t J_M(2\sqrt{\lambda x}) \right) \right],
\]

where \( e^{-\lambda} = \prod_k \cos \alpha_k; \) and \( J_M \) is a Bessel function. This leads to an analytic form for \( \chi'(\omega) \) which is plotted in Fig.1. Typically for macroscopic systems, with very large \( N, \lambda \gg 1 \), and we see that oscillations in \( P(t) \) are completely suppressed; we get strong decoherence with no dissipation. Exactly the same physical effect is obtained letting \( \alpha_k = 0 \), but adding a coupling \( 1/2\omega_0 \sum_k \vec{\alpha}_k \) (cf. (3)). To see this, we define an operator \( \hat{U}_k = \exp(i\beta_k \vec{\alpha}_k) \) which unitarily transforms the ground state \( | \vec{\alpha}_k \rangle \) of \( \vec{\alpha}_k \) in the field \( \vec{\alpha}_k \), to \( | \vec{\sigma}_k^{final} \rangle \) in \( \vec{\sigma}_k^{final} \). Then \( \beta_k = \omega_0 / 2\Omega_0, \) and \( P(t) \) has the same form as (3), except that \( e^{i\alpha_k \vec{\alpha}_k \cdot \vec{\sigma}_k} \) is replaced by \( \hat{U}_k \) in
In the final answer we need only replace $\lambda$ with $\kappa$, $e^{-\kappa} = \prod_k \cos \beta_k$.

Why is the physics of decoherence in spin baths so different from that for oscillator baths? To answer this, consider when we may reduce (2) to (1). Clearly, the mapping of an arbitrary environment to the oscillator bath can be justified when the coupling is small, and the collective coordinate is a weak perturbation to the bath. In our case it would require (a) that $\phi_k$, $\alpha_k$, and $\xi_k$ be zero, and (b) the correspondence $c_k = \omega^\|_k$, $\Omega_k = \omega^\perp_k$, and the weak coupling condition $\omega^\|_k \ll \omega^\perp_k$. The Caldeira-Leggett spectral function becomes

$$J(\omega) = \frac{\pi}{2} \sum_k \frac{c^2_k}{m_k \Omega_k} \delta(\omega - \Omega_k) \sim \frac{\pi}{2} \sum_k \frac{(\omega^\|_k)^2}{\omega^\perp_k} \delta(\omega - \omega^\perp_k)$$

(12)

The above conditions are physically incorrect for the spin bath, particularly if hyperfine couplings to nuclei are involved (the discussion for SQUID’s, where they are not involved, will be given elsewhere). Usually $\omega^\|_k > \omega^\perp_k$, and neither are small compared to, e.g., $\Delta_0$. Moreover, as we have seen, the spin bath modes are often strongly disturbed by the macroscopic coordinate (so a perturbative treatment is no longer useful), and in fact the spectrum of the spin environment is often largely defined by the coupling to the macroscopic coordinate - it would be quite different in the absence of this coupling (the hyperfine interaction provides a good example of this). Another indication of the radical difference between the two baths is shown by comparing the $M = 0$ and $M = 2$ spin bath states, which are adjacent in energy; nevertheless $P_{M=0}(t)$ and $P_{M=2}(t)$ are quite different. No such difference is possible for oscillator bath states which are neighbours in energy, and we do not see how an oscillator bath model can reproduce forms like (13). Thus in dealing with the spin bath, we deal with a new “universality class” of quantum environments, in which functions like $J(\omega)$ simply cannot meaningfully be defined.

Even if $\omega^\|_k \ll \omega^\perp_k$, the spin bath $\rightarrow$ oscillator bath mapping requires $\phi_k = \alpha_k = \xi_k = 0$. However the spin-boson model can be extended to include terms like $\sum_k (c^\dagger_k x_k + c_k^\dagger \tilde{\tau}_y x_k)$; these correspond to (2) if $c^\dagger_k = \xi_k \Delta_0$ and $c_k^\dagger = \alpha_k \Delta_0$, provided the $c^\dagger_k$, $c_k$, $\Delta_0$, the usual assumption of a continuous form for $J(\omega)$ will be invalid. It would be more usual to find a set of $\delta$-function groups in $J(\omega)$, and it might be interesting to study such a model, provided a realistic example could be found.

(iv) Quantum Measurements: Measurement theory gives another perspective on the difference between the 2 baths. In typical oscillator bath models, decoherence proceeds via exchange of quanta between the system and individual oscillators. In this way the oscillators...
perform "measurements" on the system, via interactions which distinguish between the relevant system states (e.g., in Fig.1), the coupling in the bath is proportional to $\tilde{r}_z$, and so it destroys coherence between the eigenstates $|\uparrow\rangle$ and $|\downarrow\rangle$ of $\tilde{r}_z$. This measurement is dissipative and thermodynamically irreversible.

In spin baths decoherence proceeds even if the bath energy is unaltered - the decoherence is primarily through the phase change occurring in the environmental wavefunction. Such pure phase decoherence has been previously discussed in the context of abstract models of system-environment interactions; however as far as we know, no attempt has ever been made to discuss how such decoherence might occur in the real world. We note in passing that in measurement theory we may think of the environmental spins as "inverse Stern-Gerlach measuring devices" in which now the microscopic spins observe (and thereby decohere) the macroscopic variable, instead of vice-versa.

(vi) Other implications: Spin baths are important in nature because nuclear spins are everywhere - all elements except He have significant naturally-occurring fractions of finite-spin nuclear isotopes. Moreover any reasonable number $N$ of nuclear spins coupled to a macroscopic coordinate will cause strong decoherence (see Fig.1); in fact, as $N \to \infty$, the nuclear spin bath will dominate over any oscillator bath, no matter how weak are the couplings to the nuclei. Nor should one neglect paramagnetic electronic impurities, particularly in insulators - in all but ultrapure solids, they have an important effect because their coupling to macroscopic coordinates is much stronger then that of nuclei (since $\gamma_e \gg \gamma_N$).

It is thus clear that this new class of "quantum environments" must play an important role in attempts to push back the "F.A.P.P." barrier between quantum and classical phenomena, towards the macroscopic realm. In many cases (particularly in magnetic systems), nuclear and paramagnetic spins will be the F.A.P.P. barrier to attempts to see coherence, on anything beyond the mesoscopic scale.

Finally, we hope the spin bath model may be of some use in condensed matter physics. Oscillator bath models have been usefully applied to many of the classic "many body problems", such as the X-ray edge and Kondo models, to metals, Fermi liquids, and Luttinger liquids, as well as superfluids, superconductors, and magnets. However some systems have resisted such descriptions; good examples are heavy fermions and quantum spin glasses, where multi-spin correlations are important - such correlations are not so easily bosonized. We hope to return to this question at a later time.

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