I. INTRODUCTION

A new era of quantum information processing experiments is beginning (e.g. 1, 2, 3) with the consequence that battling decoherence (the destruction by environmental degrees of freedom of the phase coherence between superposed quantum states) has become a crucial task for designing the fault-tolerant quantum computer 4. The engineering significance now attaching to decoherence gives new urgency to an already fundamental theoretical question (e.g. 2, 3, 4): what is the effect of an environmental heat bath on a quantum two-level system (qubit)?

As well as its importance for the experimental realization of a qubit 2, 3, 10, the current interest in this problem is due to at least two other factors. One is its general importance as a testbed for competing conceptions of dissipative quantum mechanics 11, 12. A second is the bridge it offers between quantum and classical stochastic systems, for example as a quantum rather than classical two level stochastic resonance system (e.g. 6, 13).

A particularly well-studied framework for the problem is the spin-boson Hamiltonian (e.g. 2, 4) in which the two level system is modelled by a spin, the environmental heat bath by quantum harmonic oscillators, and the spin is coupled to each bath oscillator independently. This Hamiltonian is easily adaptable to the driven spin-boson case where the two level system is subjected to an external force. In the strong coupling and high temperature bath limits much progress has been made, especially for the case of harmonic driving which defines the quantum stochastic resonance problem 6, 12. Hartmann et al. 14 have, however, recently emphasized that weak coupling and low temperatures remain much less well explored, and that although formal solutions for the resulting spin dynamics do now exist, they still in practise have to be used perturbatively.

Hartmann et al. 14 sought to make progress by pointing out similarities of the driven spin boson problem to counterparts in quantum optics and solid state physics where Bloch-Redfield equations are used. They exhibited a set of Bloch-Redfield equations (their Eqn. 4) obtained by projection operator methods.

In this Paper we show that an earlier path integral-based derivation of a similar set of equations 14 for the time independent spin-boson Hamiltonian can be extended to the driven case (see also 11). This allows us to derive (section III) an exact integro-differential evolution equation for the propagator of the reduced density matrix, and is the first of of three principal results of the Paper. We then (section IV) make the weak coupling assumption to give an independent derivation of a set of Bloch-Redfield equations for the driven spin boson case; the second main result of the Paper. We note in passing that this refutes the assertion by Zhang 17 that the methodology used in 16 was unsuitable for time dependent problems.

We choose an initial condition in which the environment equilibrates about a fixed spin, which is subsequently released at time $t_0$. We find, in consequence, a difference from the Bloch-Redfield equations of 14, but only in the terms arising from dissipation. This difference disappears if we follow previous authors in assuming spin and bath to be completely uncoupled at $t_0$. In either case
spectral density
dissipative LZS problem may aid study of topical issues
weak damping case, which greatly simplifies the dissipa-
tions we have derived to the LZS problem in the ohmic
mediate speeds of passage, which disagree with those of
ionally following
[21] these benefit from the recent feasibility of computa-
and computational methods (e.g. [8, 20, 21]). In one case
mer [18] has since been supplemented by other analytic
study of of the dissipative LZS problem by Ao and Ram-
vironment consisting of harmonic oscillators. The initial
tion (based on [5, 15, 26]). In subsection II A we write
the LZS Hamiltonian with a fixed tunnelling term and
additional examples). In the present case we will take
Zener-Stuckelberg (LZS) nonadiabatic level crossing
problems are found in atomic collisions, chemical
action kinetics, biophysics, solar neutrino oscillations
and NMR (see Ao and Rammer [13] for references and
additional examples). In the present case we will take
the LZS Hamiltonian with a fixed tunnelling term and
linearly time-varying bias, and study the effects of an en-
tvironment consisting of harmonic oscillators. The initial
study of of the dissipative LZS problem by Ao and Ram-
mer [13] has since been supplemented by other analytic
and computational methods (e.g. [3, 21, 22]). In one case
[21] these benefit from the recent feasibility of computa-
tionally following $\approx 120000$ basis states; but they have
all given results for the influence of the bath, for inter-
mediate speeds of passage, which disagree with those of
[18]. Here we specialize the Bloch-Redfield equa-
tions we have derived to the LZS problem in the ohmic
weak damping case, which greatly simplifies the dissipa-
tion term (as also found by [17]). These equations for the
dissipative LZS problem may aid study of topical issues
such as the merits of different models of the noise power
spectral density $J(\omega)$ of the heat bath [8] or of alter-
native functional forms for the time dependent bias in the
LZS problem (c.f. Chapter 6 of [22]).

By scaling the Bloch-Redfield equations to the char-
acteristic tunnelling time, we show that dissipation is
significant even at zero temperature, for finite speeds of
passage, agreeing with newer authors, but that its im-
pact is inversely proportional to the passage speed. This
implies the intuitively reasonable conclusion that qubits
need to be switched as fast as possible to minimise dis-
sipation effects. We illustrate our findings numerically,
in the zero temperature case where the fluctuating force
terms greatly simplify in addition to the more general
ohmic simplification of the dissipation term. Damping is
clearly seen, reminiscent of that seen for the high tem-
perature case in [19].

II. EXACT INTEGRO-DIFFERENTIAL
EVOLUTION EQUATION FOR SPIN
PROPAGATOR OF DRIVEN SPIN-BOSON
HAMILTONIAN WITH EQUILIBRIUM FIXED
SPIN INITIAL CONDITION

First, in subsection II A we describe the driven spin-
bozon system, defining the Hamiltonian and our nota-
tion (based on [3, 13, 20]). In subsection II B we write
down the reduced spin density matrix as a path integ-
ral, to which (subsection II C) we apply the equilibrium
fixed spin initial condition. We can then (subsection II D
and II E) integrate out the bath variables to find the effect
of the bath on the spin by means of the Feynman-Vernon
influence functional for this initial condition. This en-
ables us to generalize the results of Waxman [15] to the
driven spin boson case, arriving at our first main result
(II F), a general time evolution integro-differential equa-
tion for the propagator $K$ of the reduced density matrix
$\bar{\rho}$.

In this section we make only two main assumptions
in addition to those of the spin-boson model itself: i) the
widely-employed (e.g. [18]) choice of a factorizing
initial density matrix and ii) use of an “equilibrium fixed
spin” initial condition where the spin is assumed to be
fixed “up” and in equilibrium with the bath at $t_0$. To aid
subsequent comparison with Hartmann et al. [14] we also
give the equivalent influence function for the case when
spin and bath are uncoupled at $t_0$.

A. The Driven Spin Boson problem

The driven spin-boson Hamiltonian $H$ is:

$$H = H_S + H_I + H_B$$

where

$$H_S = -\frac{\hbar \Delta}{2} \sigma_x + \frac{\hbar \epsilon(t)}{2} \sigma_z$$

$$H_I = \sum_\alpha \frac{q_0}{2} \sigma_z c_\alpha x_\alpha$$

$$H_B = \sum_\alpha \left( \frac{p_\alpha^2}{2m_\alpha} + \frac{m_\alpha}{2} x_\alpha^2 \omega_\alpha^2 \right)$$

where $\sigma_i$ with $i = x, y, z$ are Pauli spin operators; $-\Delta$ and
$\epsilon(t)$ are angular frequencies corresponding to off-diagonal
(tunnelling) and on-diagonal (bias) spin matrix elements
respectively; and the bath heat is represented by a set of
harmonic oscillators of mass $m_\alpha$, angular frequency $\omega_\alpha$,
momentum $p_\alpha$ and position coordinate $x_\alpha$. The oscilla-
tors are coupled independently to the spin co-ordinate
with strength measured by the set $\{c_\alpha\}$ while $q_0$ mea-
sures the distance between the left and right potential
wells.

In contrast to most previous work (e.g. [15]) we will
use an initial condition where at times $-\infty$ to $t_0$ the spin
has been held fixed and the heat bath has equilibrated
around it: a choice which requires explanation. For
reasons of mathematical simplicity we want a factorizing
initial full density matrix. Given this, we have selected
what we believe to be the boundary condition that avoids
unnatural transients associated with the time evolution
of the complete system after $t_0$. Any other choice for the
bath’s initial density matrix would be expected to lead
cancels with its equivalent in the partition function (the denominator of (15)).

B. The density matrix as a path integral

We follow the method of [15] but the driven spin-boson Hamiltonian \( H \) replaces the static spin-boson Hamiltonian given as his equation (1). We start by expressing the density matrix of the combined system as a double path integral. The density operator \( \rho \) obeys \( i\hbar \partial \rho / \partial t = [H, \rho] \), so its time evolution is given by \( \rho(t) = U(t, t_0)\rho(t_0)U^{-1}(t, t_0) \) with \( U \) a unitary time evolution operator.

Hence with \( |x\sigma> \) an eigenstate of the oscillators’ coordinate operators \( x \) and the spin operator \( \sigma \), we have

\[
\langle x_1\sigma_1|\rho(t)|x_2\sigma_2 \rangle = \rho(x_1\sigma_1, x_2\sigma_2; t) = \sum_{\sigma_3} \sum_{\sigma_4} \int dx_3 \int dx_4 < x_1\sigma_1|U(t, t_0)|x_3\sigma_3 > < x_3\sigma_3|\rho(t_0)|x_4\sigma_4 > < x_4\sigma_4|U^{-1}(t, t_0)|x_2\sigma_2 >
\]

(6)

where we have inserted two complete sets of states and boldface type distinguishes a state of all \( N \) oscillators \( \{x, \sigma \} \). We now assume that the initial density matrix factors into an oscillator dependent part and a spin dependent part. We are only interested in the behaviour of the spin so work with the reduced density matrix, obtained by integrating over the bath variables. We then define the reduced density matrix \( \bar{\rho} \) by tracing over the bath variables, and normalizing to the free oscillator partition function. We have

\[
\bar{\rho}(\sigma_1\sigma_2t) = \sum_{\sigma_3} \sum_{\sigma_4} K(\sigma_1\sigma_2t|\sigma_3\sigma_4t_0)\bar{\rho}(\sigma_3\sigma_4t_0).
\]

(7)

Our initial problem is to determine the propagator \( K \):

\[
K(\sigma_1\sigma_2t|\sigma_3\sigma_4t_0) = \int dx' \int dx_3 \int dx_4 < x'\sigma'1|U(t, t_0)|x_3\sigma_3 > \rho(x_3\sigma_3, t_0)\bar{\rho}(x_4\sigma_4, t_0)\rho(x_4\sigma_4, t_0)\bar{\rho}(x_3\sigma_3, t_0) < x_4\sigma_4|U^{-1}(t, t_0)|x_2\sigma_2 >
\]

(8)

the effective time evolution operator for the reduced density matrix.

We now write the matrix element of the time evolution operator \( U(t, t_0) \) (the forward propagator) as a path integral

\[
\langle x_1\sigma_1|U(t, t_0)|x_3\sigma_3 \rangle = \int_{x_{t_0}}^{x_t} d[x] \int_{\sigma_{t_0}}^{\sigma_t} d[\sigma] \exp \left( \frac{i}{\hbar} S[\sigma, x] \right)
\]

(9)

with

\[
S[\sigma, x] = S_S[\sigma] + S_I[\sigma, x] + S_B[x]
\]

(10)

where \( S_S, S_I, S_B \) are the actions corresponding to the spin, interaction and bath Hamiltonian operators \( H_S, H_I \) and \( H_B \) respectively. The notation

\[
\int_{x_{t_0}}^{x_t} d[x]
\]

(11)

means the sum over all paths beginning at \( x_2 \) at time \( t_0 \) and ending at \( x_1 \) at time \( t \), and the spin path integral is explained more fully below.

Combining the above with a similar expression for the backward propagator and with the initial bath density matrix we obtain

\[
K(\sigma_1\sigma_2t|\sigma_3\sigma_4t_0) = \int_{\sigma_{t_0}}^{\sigma_t} d[\sigma] \int_{\sigma_{t_0}}^{\sigma_t} d[\nu] A_n[\sigma] A_n^*[\nu] F[\sigma, \nu]
\]

(12)

where
is the influence functional containing all effects of the bath on the spin system.

\[
F[\sigma, \nu] = \int d\sigma' \int dx_3 \int dx_4 \int dx_{4t} \int dx_{4t} \int dx_{4t} \int dx_{4t} d[y] \int dx_{t0} \int dx_{t0} \int dx_{t0} \int dx_{t0} d[x] \\
\times e^{i(S_1[\sigma, x] - S_1[\nu, y] + S_2[x] - S_2[y])} \rho(x_3 x_4 t_0)
\]

(13)

with the sum\(\sum\) running over all numbers of flips (points at which \(\sigma\) goes from \(-1\) to \(+1\) or vice versa) consistent with the initial conditions, defines both the measure \(d[\sigma]\) and the amplitude \(A_n[\sigma]\) associated with a path \([\sigma]\) containing \(n\) spin flips.

C. Application of equilibrium fixed spin initial condition

We now calculate the influence functional and so have to specify \(\rho(x_3 x_4 t_0)\), which corresponds physically to the description of the oscillator bath at time \(t_0\). We assume thermal equilibrium so

\[
\rho(x_3 x_4 t_0) = \frac{\rho(x_3 e^{-\beta H_0} x_4)}{Z_0}
\]

in which \(H_0\) denotes \(H(t = t_0)\). The partition function is given by \(Z_0 = \text{Tr} e^{-\beta H_0}\) and the inverse temperature by \(\beta = \frac{1}{k_B T}\).

We find that the path integral part of the influence functional \([13]\) factors into a product of terms like

\[
\int_{x_3 t_0}^{x_3 t_0} d[y] \int_{x_3 t_0}^{x_3 t_0} d[x] \exp \left( \frac{i}{\hbar} (S_{aI}[\sigma, x] - S_{aI}[\nu, y] + S_{aB}[x] - S_{aB}[y]) \right)
\]

(16)

one for each \([\square]\) oscillator, \(x_3\) and \(x_4\) are the initial states for the forward and backward paths. Noting that the (single particle) bath and interaction actions are

\[
S_{aI}[\sigma, x] + S_{aB}[x] = \int_{t_0}^{t} du \left( \frac{m_\alpha x_\alpha^2}{2} - \frac{m_\alpha \omega_\alpha^2 x_\alpha^2}{2} - \frac{c_\alpha x_\alpha g_0 \sigma}{2} \right)
\]

(17)

we first evaluate the forward propagator for the bath variables, a standard result \([23]\):

\[
\int_{x_3 t_0}^{x_3 t_0} d[x] \exp \left( \frac{i}{\hbar} (S_{aI}[\sigma, x] + S_{aB}[x]) \right) = \left( \frac{m_\alpha \omega_\alpha}{2 \pi i \hbar \sin \omega_\alpha (t - t_0)} \right)^{\frac{1}{2}}
\]

\[
\times \exp \left( \frac{im_\alpha \omega_\alpha}{2 \hbar \sin \omega_\alpha (t - t_0)} B \right)
\]

(18)

with

\[
B = (x_3^2 + (x')^2) \cos \omega_\alpha (t - t_0) - 2x' x_3
\]

\[-x' f_\sigma (t - t_0) + x_3 g_\sigma (t - t_0)\]
We note that the above expressions depend on the sign of the coupling constant where \( f \) and the functions \( h \) hence the use of the \( \alpha \) index. We now do the integral over \( 0 \leq x' \leq t \), which yields a delta function, so the path integral part of the influence functional becomes

\[
\int_{x_3 \leq t_0}^x d[x] \int_{x_4 \leq 0}^{x'} d[y] \exp \left[ \frac{i}{\hbar} (S_{\alpha I}[\sigma, x] - S_{\alpha I}[\nu, y] + S_{\alpha B}[x] - S_{\alpha B}[y]) \right] = \left( \frac{m_{\alpha \omega_\alpha}}{2\pi \hbar \sin \omega_\alpha(t - t_0)} \right) \exp \left( \frac{im_{\alpha \omega_\alpha}}{2\hbar \sin \omega_\alpha(t - t_0)} C \right)
\]

where

\[
C = (x_3^2 - x_4^2) \cos \omega_\alpha(t - t_0) - 2x'(x_3 - x_4) - x'[f_\sigma(t - t_0) - f_\nu(t - t_0)] + x_3g_\sigma(t - t_0) - x_4g_\nu(t - t_0)
\]

\[
- \frac{c_\alpha g_0}{m_{\alpha \omega_\alpha}} \int_{t_0}^t du \int_{t_0}^u dv \times [\sigma(u)\sigma(v) - \nu(u)\nu(v)] \sin \omega_\alpha(t - u) \sin \omega_\alpha(v - t_0)
\]

and the functions \( f_\nu, g_\nu \) are \( f_\sigma, g_\sigma \) but with \( \nu(u) \) replacing \( \sigma(u) \). All of the above is still just for one oscillator hence the use of the \( \alpha \) index. We now do the integral over \( x' \) in equation (13), which yields a delta function, so the path integral part of the influence functional becomes

\[
\int_{x_3 \leq t_0}^x d[x] \int_{x_4 \leq 0}^{x'} d[y] \exp \left[ \frac{i}{\hbar} (S_{\alpha I}[\sigma, x] - S_{\alpha I}[\nu, y] + S_{\alpha B}[x] - S_{\alpha B}[y]) \right] = X \delta \left[ \frac{X}{2} (2(x_3 - x_4) - (f_\sigma - f_\nu)) \right] \exp \left( \frac{iX}{2} D \right),
\]

where

\[
X = \frac{m_{\alpha \omega_\alpha}}{\hbar \sin \omega_\alpha(t - t_0)}
\]

and

\[
D = (x_3^2 - x_4^2) \cos \omega_\alpha(t - t_0) + x_3g_\sigma(t - t_0) - x_4g_\nu(t - t_0)
- \frac{c_\alpha g_0}{m_{\alpha \omega_\alpha}} \int_{t_0}^t du \int_{t_0}^u dv \times [\sigma(u)\sigma(v) - \nu(u)\nu(v)] \sin \omega_\alpha(t - u) \sin \omega_\alpha(v - t_0).
\]

We note that the above expressions depend on the sign of the coupling constant \( c_\alpha \) via the \( f_{\sigma,\nu} \) and \( g_{\sigma,\nu} \) terms, but
not the initial value of \( \sigma \) (because \( \mathcal{F}_\alpha \) is a product of two propagators). The initial value we chose for \( \sigma, (= + q_0 / 2) \) did, however, appear in the thermalized density matrix for the bath.

We recall from (13) and (15) the full influence functional including all the oscillators. The path integrals factor similarly, so \( \int \mathcal{D}x \mathcal{D}t \mathcal{D}x' \mathcal{D}t' \) is a product of single particle path integrals over all paths that the individual \( x_\alpha \) can follow consistent with the set \( \{ x_\alpha \} \) being \( x' \) at time \( t \), and \( x_3 \) at \( t_0 \). If we can “fold” in the product of the traces of single-particle propagators given by (23) and (25) we can then multiply by \( \rho(x_3,x_4,t_0) \) and do the integrals over \( x_3 \) and \( x_4 \) to obtain the influence functional.

\[
F_\alpha[\sigma,\nu] = \int dz_1 dz_2 \delta \left( z_1 - \frac{1}{2}(f_\sigma - f_\nu) \right) <z_1 + \frac{z_2}{2} e^{-\beta H_{\alpha}}|z_1 - \frac{z_2}{2}> \\
\times \exp \left( \frac{im_\alpha \omega_\alpha}{2\hbar \sin \omega_\alpha(t - t_0)} M \right)
\]

and

\[
M = z_1(f_\sigma - f_\nu) \cos \omega_\alpha(t - t_0) + z_1(g_\sigma - g_\nu) + \frac{z_2}{2}(g_\sigma + g_\nu) \\
- \frac{e^2 q_0^2}{m_\alpha^2 \omega_\alpha^2} \int_t^{t_0} du \int_{t_0}^u dv
\]

where the delta function has been used to replace \( x_3^2 - x_4^2 \) by \( z_1(f_\sigma - f_\nu) \). We now consider

\[
<z_1 + \frac{z_2}{2} e^{-\beta H_{\alpha}}|z_1 - \frac{z_2}{2}> = \frac{\rho_{osc}}{Z_0} (z_1 + z_2/2 + A, z_1 - z_2/2 + A)
\]

If we now write \( z_1 + A = z_1' \) we get

\[
F_\alpha[\sigma,\nu] = F_{\alpha A=0}[\sigma,\nu] \exp (P)
\]

with

\[
P = \frac{im_\alpha \omega_\alpha}{2\hbar \sin \omega_\alpha(t - t_0)} (-A) [ (f_\sigma - f_\nu) \cos \omega_\alpha(t - t_0) + (g_\sigma - g_\nu) ],
\]

and \( F_{\alpha A=0} \) the conventional influence function.

**D. Evaluation of the influence functional in equilibrium fixed spin case**

We want to evaluate a non-standard influence functional, corresponding to the equilibrium fixed spin initial condition. We do so by replacing it by the influence functional for a system with the spin and bath uncoupled at \( t_0 \) multiplied by a phase due to the fixed spin boundary condition. To derive this result we now go to sum and difference coordinates \( z_1 = \frac{z_3 + z_4}{\sqrt{2}} \) and \( z_2 = x_3 - x_4 \).

If we define \( F_\alpha[\sigma,\nu] \), the single oscillator influence functional, by \( F[\sigma,\nu] = \prod_\alpha F_\alpha[\sigma,\nu] \), then using (13), and \( H_{\alpha 0} \) of the form given in (5), we have
\[-\frac{c_\alpha q_0}{m_\alpha \omega_\alpha} \int_{t_0}^t du [\sigma(u) - \nu(u)] \sin \omega_\alpha (t - t_0) \cos \omega_\alpha (u - t_0)\]

so the full influence functional is

\[
F[\sigma, \nu] = \left( \prod_\alpha F_{\alpha A=0} \right) \exp \sum_\alpha \frac{ic_\alpha q_0}{2\hbar} A \int_{t_0}^t du [\sigma(u) - \nu(u)] \cos \omega_\alpha (u - t_0)
\]

\[
= F_{A=0} \exp \frac{iq_0^2}{4\hbar} \sigma(t_0) \int_{t_0}^t du [\sigma(u) - \nu(u)] 2Q_1(u - t_0)
\]

(33)

where

\[
F_{A=0} = \prod_\alpha F_{\alpha A=0},
\]

(34)

is the bath spectral function describing the oscillator heat bath. Equation (33) should be compared with the expression arrived at by Leggett et al. as their equations (B.1.9) and (B.1.10). All we need now is the standard result

\[
F_{A=0}[\sigma, \nu] = \exp -\frac{iq_0^2}{4\hbar} \int_{t_0}^t du \int_{t_0}^u dv [\sigma(u) - \nu(u)][\sigma(v) + \nu(v)] Q_1' (u - v)
\]

\[
\times \exp -\frac{q_0^2}{4\hbar} \int_{t_0}^t du \int_{t_0}^u dv [\sigma(u) - \nu(u)][\sigma(v) - \nu(v)] Q_2(u - v)
\]

(37)

where \(\tau = \beta \hbar\). We also have the conventionally defined correlation function \(Q_2\) for the fluctuating force (see also Appendix B) and the retarded resistance function \(Q_1'\) (see [7]) given by

\[
Q_2(u) = \int_0^\infty \frac{d\omega}{\pi} J(\omega) \coth \frac{\omega \tau}{2} \cos \omega u,
\]

(38)

\[Q_1'(u) = \frac{d}{du} Q_1(u)\]

respectively. The propagator for the reduced spin density matrix in (12) becomes

\[
K(\sigma_1 \sigma_2 \sigma_3 \sigma_4 | t) = \int_{\sigma_3 t_0}^{\sigma_1 t} d[\sigma] \int_{\sigma_4 t_0}^{\sigma_2 t} d[\nu] A_\alpha [\sigma] A_\alpha^* [\nu] F[\sigma, \nu]
\]

\[
= \int_{\sigma_3 t_0}^{\sigma_1 t} d[\sigma] \int_{\sigma_4 t_0}^{\sigma_2 t} d[\nu] A_\alpha [\sigma] A_\alpha^* [\nu] F_{A=0}[\sigma, \nu]
\]
\[ \times \exp \left( \frac{i q_0^2}{2 \hbar} \sigma(t_0) \right) \int_{t_0}^{t} du Q_1(u - t_0) [\sigma(u) - \nu(u)]. \] (40)

We see that the equilibrium fixed spin initial condition has altered only the imaginary (dissipative) first factor in equation 7 of [12], Waxman’s expression for the influence functional. The second (real) factor due to fluctuations is unchanged.

E. Simplification of the fixed spin influence functional

We can simplify the first part of the influence functional considerably by using the extra factor introduced by the spin boundary condition. From (37) and (33) we have:

\[
F[\sigma, \nu] = \exp \left\{ \frac{i}{\hbar} \sigma(t_0) \left( \frac{q_0}{2} \right)^2 \int_{t_0}^{t} du [\sigma(u) - \nu(u)] 2Q_1(u - t_0) \right\} \\
\times \exp \left\{ - \frac{i q_0^2}{4 \hbar} \int_{t_0}^{t} du \int_{t_0}^{u} dv [\sigma(u) - \nu(u)] \left[ \sigma(v) + \nu(v) \right] Q_1'(u - v) \right\} \\
\times \exp \left\{ - \frac{q_0^2}{4 \hbar} \int_{t_0}^{t} du \int_{t_0}^{u} dv [\sigma(u) - \nu(u)] \left[ \sigma(v) - \nu(v) \right] Q_2(u - v) \right\}. \] (41)

We note that

\[
\int_{t_0}^{u} dv [\sigma(v) + \nu(v)] Q_1'(u - v) - 2Q_1(u - t_0)\sigma(t_0) = -[\sigma(u) + \nu(u)]Q_1(0) + \int_{t_0}^{u} dv \frac{d}{dv} [\sigma(v) + \nu(v)]Q_1(v - u) \] (42)

since \( \sigma(t_0) = \nu(t_0) = 1 \). Now

\[
\int_{t_0}^{t} du [\sigma(u) - \nu(u)] [\sigma(u) + \nu(u)] Q_1(0) = 0 \] (43)

as \( \sigma^2(u) - \nu^2(u) \equiv 0 \), for all \( u \). Therefore the influence function reduces to

\[
F[\sigma, \nu] = \exp \left( \int_{t_0}^{t} du \int_{t_0}^{u} dv f(u, v) \right) \] (44)

with

\[
f(u, v) = - \frac{iq_0^2}{4\hbar} [\sigma(u) - \nu(u)] \frac{d}{dv} [\sigma(v) + \nu(v)] Q_1(v - u) \]

\[
- \frac{q_0^2}{4\hbar} [\sigma(u) - \nu(u)] [\sigma(v) - \nu(v)] Q_2(u - v) \] (45)

which may be compared to equation 7 of [13].

We note (see also the appendix B) that the second factor of (45) can be viewed as the effect of a classical fluctuating force. We will specialise later to the ohmic [5] case when

\[
J(\omega) \approx \eta \omega e^{-\omega/\omega_c} \] (46)

for which \( Q_1(u) \) will be well approximated by a delta function \( \eta \delta(u) \).

We can now follow Waxman [13] by differentiating the above propagator \( K \) to obtain a differential equation for the time evolution of \( K \) differing from his equation (15) only in the replacement of \( e \) by \( e(t) \) and by the replacement of his term in \( Q_1 \) by one arising from the fixed spin.
For the driven spin-boson system with factorizing initial density matrix and equilibrium fixed spin initial condition the above integro-differential equation (47) is exact, and the first main result of this Paper.

III. BLOCH-REDFIELD EQUATIONS FOR THE WEAK DAMPING CASE

We now go on in this section (III A) to demonstrate that one may obtain a simpler set of equations of Bloch-Redfield form-for the spin vector $a$ by making a weak damping approximation, replacing terms under the retarded integrals of the propagator equation (47) by their equivalents for an uncoupled spin $a^{(0)}$. We then (III C) identify the dissipation term $\chi$ arising from the imaginary factor in the influence functional. In addition we identify (III D) the terms due to the fluctuating force allowing us to complete the Bloch-Redfield equations, and compare them with those of Hartmann et al. (III E).

A. Weak damping approximation

We will now approximate the terms $<\sigma(v)\pm\nu(v)>$ in (47) by their value for an undamped system i.e. $<\sigma(v)\pm\nu(v)>\approx<\sigma(v)\pm\nu(v)>_0$ This is in general a weak damping approximation. In the ohmic case it implies $\alpha\ll 1$ where $\alpha$ is the dimensionless friction constant for the problem, $\alpha = \eta q^2/2\pi \hbar$ and $\eta$ is as defined in (46). We note that linearity implies $<\sigma(v)\pm\nu(v)>_0<\sigma(v)>_0\pm<\nu(v)>_0$. Then $<\sigma(v)>_0<\sigma_1 U^{(0)}(t,v)\sigma_2 U^{(0)}(v,t_0)\sigma_3><\sigma_2 U^{(0)}(t,t_0)\sigma_4>*$ (see also equations (20) and (21) of [12]). Here $U^{(0)}$ is the time evolution operator for a spin uncoupled to the bath:

$$U^{(0)}(t_1,t_2) = T \exp \left( -\frac{i}{\hbar} \int_{t_1}^{t_2} H_S(t')dt' \right)$$  \hspace{1cm} (49)

where $T$ denotes the time-ordering operator.

Using the definition of the inverse of $U^{(0)}$ we find

$$<\sigma(v)>_0<\sigma_1\sigma_2(t,v)\sigma_3U^{(0)-1}(t,v)U^{(0)}(v,t)U^{(0)}(v,t_0)\sigma_4><\sigma_2U^{(0)}(t,t_0)\sigma_4>*$$  \hspace{1cm} (50)
but \( U^{(0)}(t, v)U^{(0)}(v, t_0) = U^{(0)}(t, t_0) \) so
\[
<\sigma(v) >_0 = \langle \sigma_1 U^{(0)}(t, v)\sigma_2 U^{(0)}(v, t)U^{(0)}(t, t_0)\sigma_3 \rangle
\]
\[
<\sigma_2|U^{(0)}(t, t_0)\rangle_4 >^* .
\]
Inserting a complete set of states of \( \sigma_z \):
\[
1 = \sum_\sigma |\sigma> <\sigma| = |+\sigma_1> + |-\sigma_1>
\]
(51)

we have:
\[
<\sigma(v) >_0 = \langle \sigma_1 U^{(0)}(t, v)\sigma_2 U^{(0)}(v, t)\sigma_1 > K^{(0)}(\sigma_1 \sigma_2 t|\sigma_3 \sigma_4 t_0)
\]
\[
+ <\sigma_1 U^{(0)}(t, v)\sigma_2 U^{(0)}(v, t)| -\sigma_1 > K^{(0)}(-\sigma_1 \sigma_2 t|\sigma_3 \sigma_4 t_0)
\]
(52)

where the superscript on \( K^{(0)} \) indicates that it propagates the uncoupled spin density matrix. If
\[
K(\sigma_1 \sigma_2 t|\sigma_3 \sigma_4 t_0) = \int_{\sigma_3 t_0}^{\sigma_1 t} d[\sigma] \int_{\sigma_4 t_0}^{\sigma_2 t} d[\nu] A_\alpha[\sigma] A^*_\alpha[\nu] F[\sigma, \nu]
\]
then
\[
K^{(0)}(\sigma_1 \sigma_2 t|\sigma_3 \sigma_4 t_0) = \int_{\sigma_3 t_0}^{\sigma_1 t} d[\sigma] \int_{\sigma_4 t_0}^{\sigma_2 t} d[\nu] A_\alpha[\sigma] A^*_\alpha[\nu] F[\sigma, \nu]
\]
(54)
i.e. the case \( F[\sigma, \nu] = 1 \) (no environment). This is important because \( K \) propagates \( \tilde{\rho}(\sigma_3 \sigma_4 t_0) \) to \( \tilde{\rho}(\sigma_1 \sigma_2 t) \) (with \( t > t_0 \)) while \( K^{(0)} \) will propagate the same \( \tilde{\rho}(\sigma_3 \sigma_4 t_0) \) to a different final density matrix which we have called \( \tilde{\rho}^{(0)}(\sigma_1 \sigma_2 t) \). Neglect of this point would lead to the appearance of terms \( O(\alpha^2) \) in the final equation of motion. We note that the propagator \( J \) in equation (22) of \( 15 \) should, in the notation of the present paper, have been written as \( J^{(0)} \).

We now want to evaluate the terms
\[
<\sigma_1 U^{(0)}(t, v)\sigma_2 U^{(0)}(v, t)\sigma_1 >.
\]
(55)

To do this consider the density operator \( \rho^{(0)}(t) \) which is the solution of
\[
\frac{\partial}{\partial t} \rho^{(0)}(t) = [H, \rho^{(0)}]
\]
(56)

Then \( \rho^{(0)}(t) = U^{(0)}(t, t_0)\rho^{(0)}(t_0)U^{(0)}(0, t) \) allowing us to form the identity \( 2\rho^{(0)}(t) - 1 = U^{(0)}(t, t_0)\{2\rho^{(0)}(t_0) - 1\}U^{(0)}(0, t) \). Defining a polarization vector \( a^{(0)}(t) \) by
\[
\rho^{(0)}(t) = \frac{1}{2}(1 + a^{(0)}(t) \cdot \sigma)
\]
we can write \( 2\rho - 1 \) as
\[
a^{(0)}(t) \cdot \sigma = U^{(0)}(t, t_0)[a^{(0)}(t_0) \cdot \sigma]U^{(0)}(0, t_0).
\]
(57)

If \( a^{(0)}(t_0) \cdot \sigma = \sigma_z \) which is the case we need in order to evaluate (55), we can then (c.f. \( 15 \)) define an auxiliary polarization vector \( f(t, t_0) \) by \( f(t, t_0) = a^{(0)}(t) \). The dependence on \( t_0 \) enters via (57). \( f(t, t_0) \) corresponds to the polarization vector for an isolated spin evolved from time \( t_0 \) to time \( t \) subject to the initial condition that its polarization vector was \( (0, 0, 1) \) at time \( t_0 \). We will later use the equivalent notation \( a^{(0)}(t_0) \) for this function, where the above initial condition is implied.

Having established the meaning of the terms \( <\sigma_1 U^{(0)}(t, v)\sigma_2 U^{(0)}(v, t)\sigma_1 > \) we are in a position to substitute the expressions for them into the equation of motion for \( K(\sigma_1 \sigma_2 t|\sigma_3 \sigma_4 t_0) \). We first note that:
\[
<\sigma_1 U^{(0)}(t, v)a^{(0)}(v) \cdot \sigma U^{(0)}(v, t)\sigma_1 > = \sigma_1 f_3(t, v)
\]
(58)

and similarly
\[
<\sigma_1 U^{(0)}(t, v)a^{(0)}(v) \cdot \sigma U^{(0)}(v, t)\sigma_1 > = f_1(t, v) - i\sigma_1 f_2(t, v)
\]
(59)

Hence equation (52) becomes:
\[
<\sigma(v) >_0 = (f_1(t, v) - if_2(t, v)\sigma_1)K^{(0)}(-\sigma_1 \sigma_2 t|\sigma_3 \sigma_4 t_0) + \sigma_1 f_3(t, v)K^{(0)}(\sigma_1 \sigma_2 t|\sigma_3 \sigma_4 t_0)
\]
(60)

This step is crucial because it allows the use of the spin polarization vectors for an uncoupled spin.

Substitution of our expression for \( \partial_t K(\sigma_1 \sigma_2 t|\sigma_3 \sigma_4 t_0) \) into the equation for \( \partial_t \tilde{\rho}(\sigma_1 \sigma_2 t) \) will now give a soluble expression for the reduced density matrix \( \tilde{\rho}(\sigma_1 \sigma_2 t) \). Using equations (7), (60) and (17) we have:
\[ i\hbar \frac{\partial}{\partial t} \tilde{\rho}(\sigma_1 \sigma_2 t) = i\hbar \frac{\partial}{\partial t} \sum_{\sigma_3 \sigma_4} K(\sigma_1 \sigma_2 t | \sigma_3 \sigma_4 t_0) \tilde{\rho}(\sigma_3 \sigma_4 t_0) \]
\[ = i\hbar \sum_{\sigma_3 \sigma_4} \partial_t K(\sigma_1 \sigma_2 t | \sigma_3 \sigma_4 t_0) \tilde{\rho}(\sigma_3 \sigma_4 t_0) \]
\[ = -\frac{\Delta}{2} \hbar [\tilde{\rho}(\sigma_1 \sigma_2 t) - \rho(\sigma_1 - \sigma_2 t)] + \epsilon(t) \frac{\hbar}{2} (\sigma_1 - \sigma_2) \tilde{\rho}(\sigma_1 \sigma_2 t) \]
\[ + \left( \frac{\hbar}{2} \sigma_1 \sigma_2 \right) \tilde{\rho}(\sigma_1 \sigma_2 t) \]
\[ \times \left| t \right| \int_{t_0}^t dv Q_1(v - t) \frac{d}{dv} \left\{ f_1(t, v) \tilde{\rho}^{(0)}(\sigma_1 \sigma_2 t) + f_1(t, v) \tilde{\rho}^{(0)}(\sigma_1 - \sigma_2 t) \right\} \]
\[ + \int_{t_0}^t dv Q_1(v - t) \frac{d}{dv} \left\{ -i f_2(t, v) (\sigma_1 \tilde{\rho}^{(0)}(\sigma_1 - \sigma_2 t) - \sigma_2 \tilde{\rho}^{(0)}(\sigma_1 - \sigma_2 t)) \right\} \]
\[ + (\sigma_1 + \sigma_2) \int_{t_0}^t dv Q_1(v - t) \frac{d}{dv} \rho^{(0)}(\sigma_1 \sigma_2 t) \]
\[ - i \int_{t_0}^t dv Q_2(t - v) \left\{ f_1(t, v) \tilde{\rho}^{(0)}(\sigma_1 \sigma_2 t) - f_1(t, v) \tilde{\rho}^{(0)}(\sigma_1 - \sigma_2 t) \right\} \]
\[ - \int_{t_0}^t dv Q_2(t - v) \left\{ f_2(t, v) \sigma_1 \tilde{\rho}^{(0)}(\sigma_1 \sigma_2 t) - f_2(t, v) \sigma_2 \tilde{\rho}^{(0)}(\sigma_1 - \sigma_2 t) \right\} \]
\[ - i(\sigma_1 - \sigma_2) \int_{t_0}^t dv Q_2(t - v) f_3(t, v) \sigma_1 \tilde{\rho}^{(0)}(\sigma_1 \sigma_2 t) + O(\alpha^2). \] (61)

**B. Identification of spin precession terms**

We note first that, after defining the reduced density operator \( \tilde{\rho}(t) \) and its corresponding polarization vector \( a(t) \) through
\[ \tilde{\rho}(\sigma_1 \sigma_2 t) = \langle \sigma_1 | \tilde{\rho} | \sigma_2 \rangle = \langle \sigma_1 | (1 + a(t) \cdot \sigma) | \sigma_2 \rangle. \] (62)

the terms in \( \Delta \) and \( \epsilon(t) \) on the right of (61) will give the familiar spin precession term
\[ \frac{\partial a}{\partial t} = b(t) \wedge a + \ldots \] (63)

We have also defined \( b(t) = (-\Delta, 0, \epsilon(t)) \) so that
\[ H_S = \frac{\hbar}{2} b(t) \cdot \sigma. \] (64)

**C. Identification of dissipation terms**

We now consider the next three groups of terms, i.e. those in \( Q_1 \), in equation (61). These are due to dissipation and one may call them the systematic terms by analogy with the Fokker-Planck equation. The last is zero as \( (\sigma_1 - \sigma_2)(\sigma_1 + \sigma_2) = \sigma_1^2 - \sigma_2^2 \equiv 0 \) for all \( \sigma_1, \sigma_2 \) (remember \( \sigma_i = \pm 1 \) for \( i = 1, 2 \)). The first can be found by forming commutators:

\[ \langle \sigma_1 - \sigma_2 | \tilde{\rho}^{(0)}(\sigma_1 - \sigma_2 t) + \tilde{\rho}^{(0)}(\sigma_1 - \sigma_2 t) \rangle = \langle \sigma_1 | [\sigma_z, \tilde{\rho}^{(0)}(t)] | \sigma_2 \rangle \]
\[ + \langle \sigma_1 | [\sigma_z, \tilde{\rho}^{(0)}(t) \sigma_z] | \sigma_2 \rangle. \] (65)

Now \( \tilde{\rho}^{(0)}(t) = \frac{1}{2}(1 + a^{(0)}(t) \cdot \sigma) \) so the above expression becomes \( \langle \sigma_1 | 2i a \sigma_y | \sigma_2 \rangle \). Similarly the second term gives \(-i(\sigma_1 - \sigma_2) \langle \sigma_1 \tilde{\rho}(\sigma_1 \sigma_2 t) - \sigma_2 \tilde{\rho}(\sigma_1 - \sigma_2 t) \rangle = \langle \sigma_1 | 2i a \sigma_y | \sigma_2 \rangle \).
we then have of the Bloch-Redfield equations for this initial condition. and defining a vector \( \mathbf{f} \) the auxiliary vector \( \mathbf{f} \) is a unit vector in the \( y \) direction then \( \mathbf{\sigma} \cdot \mathbf{e}_y = \sigma_y \) etc., and we substitute these values into equation (61) and use (62)

\[
\frac{i\hbar}{\partial t} \mathbf{a} \cdot \mathbf{\sigma} = \ldots
\]

\[
+ \left( \frac{g_0}{2} \right)^2 \int_{t_0}^t dv \ Q_1(t - v) 2i \{ f_y'(t, v) \sigma_y - f_2'(t, v) \sigma_x \}
\]

\[
+ \ldots
\]

(66)

where we have used the evenness of \( Q_1(u) \equiv Q_1(-u) \). If \( e_y \) is a unit vector in the \( y \) direction then \( \mathbf{\sigma} \cdot \mathbf{e}_y = \sigma_y \) etc., and defining a vector \( \mathbf{f} \) by

\[
\mathbf{f}'(t, v) = (f_1', f_2', f_3') = \frac{d}{dv} \mathbf{f}(t, v)
\]

we then have

\[
\frac{\partial \mathbf{a}}{\partial t} = \mathbf{b}(t) \wedge \mathbf{a} + \chi + \ldots
\]

with

\[
\chi = \frac{4}{\hbar} \left( \frac{g_0}{2} \right)^2 \int_{t_0}^t dv \ Q_1(t - v) \mathbf{e}_z \wedge \mathbf{f}'(t, v).
\]

This completes the derivation of the dissipative part of the Bloch-Redfield equations for this initial condition.

\[
- i(\sigma_1 - \sigma_2)[\sigma_1 \hat{\rho}^{(0)}(0) - \sigma_1 \sigma_2 t] + \sigma_2 \hat{\rho}^{(0)}(\sigma_1 - \sigma_2 t) = \langle \sigma_1 | - 2\sigma_y a^{(0)}(t) | \sigma_2 \rangle
\]

(71)

while

\[
(\sigma_1 - \sigma_2)^2 \hat{\rho}(\sigma_1 \sigma_2 t) = \langle \sigma_1 | (2 \sigma_x a^{(0)}_x(t) + 2 \sigma_y a^{(0)}_y(t) | \sigma_2 \rangle.
\]

(72)

If we substitute these values into equation (61) and use the auxiliary vector \( \mathbf{f} \) we find that the equation of motion for \( \mathbf{a}(t) \) is:

\[
\frac{\partial \mathbf{a}}{\partial t} = \mathbf{b} \wedge \mathbf{a}
\]

\[
+ \frac{4}{\hbar} \left( \frac{g_0}{2} \right)^2 \int_{t_0}^t dv \ Q_1(t - v) \mathbf{e}_z \wedge \mathbf{f}'(t, v)
\]

\[
+ \mathbf{e}_z \wedge \frac{4}{\hbar} \left( \frac{g_0}{2} \right)^2 \int_{t_0}^t dv \ Q_2(v - t) \mathbf{f}(t, v) \wedge \mathbf{a}^{(0)}(t)
\]

\[
= \mathbf{b} \wedge \mathbf{a} + \chi - \mathbf{e}_z \wedge (\psi(t) \wedge \mathbf{a}^{(0)}) + O(\alpha^2)
\]

(73)

and similarly for \( f'_2 \) and \( f'_3 \) we have

\[
\frac{d}{dv} f_1(t, v) = f_1'(t, v)
\]

D. Identification of fluctuating force terms

We finally have the group of terms in \( Q_2 \) from equation (62). First

\[
\langle \sigma_1 - \sigma_2 \rangle (\hat{\rho}^{(0)}(0) - \sigma_1 \sigma_2 t) - \hat{\rho}^{(0)}(\sigma_1 - \sigma_2 t))
\]

\[
= \frac{1}{2} \langle \sigma_1 | a_y^{(0)}(t) | \sigma_z, [\sigma_x, \sigma_y] | \sigma_2 \rangle - \frac{1}{2} \langle \sigma_1 | a_z^{(0)}(t) | \sigma_z, [\sigma_x, \sigma_y] | \sigma_2 \rangle
\]

\[
+ \frac{1}{2} \langle \sigma_1 | a_x^{(0)}(t) | \sigma_z, [\sigma_x, \sigma_y] | \sigma_2 \rangle
\]

\[
= 0 + \frac{1}{2} \langle \sigma_1 | a_z^{(0)}(t) (2t)^2 \sigma_z | \sigma_2 \rangle
\]

(70)

and similarly

\[
\psi_j = - \frac{4}{\hbar} \left( \frac{g_0}{2} \right)^2 \int_{t_0}^t dv \ Q_2(t - v) f_j(t, v)
\]

(74)

Equation (74) has been derived by omitting terms of \( O(\alpha^2) \) and higher. While this procedure seems reasonable it leads, at long times, to unreasonable results in, for example, problems where \( \mathbf{b} \) is independent of time. In these cases the \( a^{(0)} \) term continues to oscillate indefinitely, and thus the system will not tend to a time independent state of equilibrium, as we believe it should. The simple replacement of \( a^{(0)} \) by \( \mathbf{a} \) appears to cure this problem; for a static \( \mathbf{b} \) the system does equilibrate [13]. We view this as a selective resummation (to infinite order in \( \alpha \)) that is sufficient to guarantee more correct long time behaviour, which we make due to its physical reasonableness.
We thus replace $a^0(t)$ in equation (62) by $a(t)$ to give:

$$\frac{\partial a}{\partial t} = b(t) \wedge a + \chi - \hat{e}_z \wedge (\psi(t) \wedge a)$$  \hspace{1cm} (75)

Equation (75) and its derivation by path integral, with the auxiliary definitions of $\chi$ (69) and $\psi$ (74) forms the second main result of our work.

E. Comparison with Bloch-Redfield equations of Hartmann et al.

Hartmann et al. [14] quote a set of Bloch-Redfield equations obtained from projection operator methods as their equation (4):

$$\begin{pmatrix} \dot{\sigma}_x \\ \dot{\sigma}_y \\ \dot{\sigma}_z \end{pmatrix} = \begin{pmatrix} 0 & \epsilon & 0 \\ -\epsilon & 0 & \Delta \\ 0 & -\Delta & 0 \end{pmatrix} \begin{pmatrix} \sigma_x \\ \sigma_y \\ \sigma_z \end{pmatrix} + \begin{pmatrix} -\Gamma_{xx} & 0 & -\Gamma_{xz} \\ 0 & -\Gamma_{yy} & -\Gamma_{yz} \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \sigma_x \\ \sigma_y \\ \sigma_z \end{pmatrix} + \begin{pmatrix} A_x \\ A_y \\ A_z \end{pmatrix}$$  \hspace{1cm} (76)

where $\sigma_{x,y,z}$ are spin expectation values i.e. $a_{x,y,z}$ in our notation. To establish the correspondence with our work note first that they have a complex correlation function:

$$M = 1 \int_0^\infty d\omega J(\omega)[\cosh(h\omega/2kB T - i\omega t)/\sinh(h\omega/2kB T)]$$

$$= M' + iM''$$  \hspace{1cm} (77)$\alpha$

which is equivalent to $Q_2 + iQ_1'$ in our notation. They also define transition amplitudes for an uncoupled spin between right and right, and left and right, pairs of states as $U_{RR} =< R|U(t,t')|R >$ and $U_{RL} =< R|U(t,t')|L >$ respectively, and an auxiliary function $F(t) = \int_0^t dt' M'(t-t')U_{RR}(t)U_{RL}$ so that $A_x = ImF(t)$ and $A_y = ReF(t)$. Finally they have the damping tensors $\Gamma_{ij}$ defined by $\Gamma_{ij} = \int_0^t dt' M'(t-t')b_{ij}(t,t')$. If we follow Hartmann et al. by defining $b_{yz} = -2Im(U_{RR}U_{RL})$ and $b_{xz} = -2Re(U_{RR}U_{RL})$, it becomes clear that their $b_{yz}$ corresponds to our $a_0^0$ and $b_{xz}$ to our $a_0^x$.

We thus find that their $\Gamma_{xx} = \Gamma_{yy} = -\psi_z$, and also $\Gamma_{zx} = \psi_x$, $\Gamma_{yz} = \psi_y$. This gives an identical structure to ours for the fluctuating force term, while their dissipation term $A = A_x e_x + A_y e_y (\equiv \chi)$ is different, being

$$A_x \equiv -\int_{t_0}^t dt' \dot{Q}_x(t-t') a_0^0$$  \hspace{1cm} (78)

$$A_y \equiv \int_{t_0}^t dt' \dot{Q}_y(t-t') a_0^0$$  \hspace{1cm} (79)

However the difference would disappear if we were to revert to a factorizing initial condition without fixed spin. The other point to stress is that both our derivation and theirs arrive at a fluctuating force term with $a^0$, the substitution of $a$ at that point has to be an additional assumption.

IV. BLOCH-REDFIELD EQUATIONS IN THE OHMIC AND ZERO TEMPERATURE CASES

We now use the result of Waxman [15] and Zhang [17] that in the ohmic case the full expression for the time dependent $\chi$ vector (69) greatly simplifies to the time independent $\hat{e}_x$. In the critical damping case studied by Shytov [8] where $J(\omega) \sim \omega^{-1}$ both $x$ and $y$ terms would be present in $\chi$.

A. Simplification of the dissipation term for ohmic spectral function

In the ohmic case, equation (69) becomes $Q_1(u) \approx \eta_0 u$ so

$$\chi = \frac{\eta_0^2}{2\hbar} \hat{e}_x \wedge f'(t,t)$$  \hspace{1cm} (80)

where the extra factor of $1/2$ comes from the use of the delta function at an endpoint of the integral. Now

$$f'(t,t) \equiv \lim_{t' \to t} \frac{d}{dt'} f(t',t) = b \wedge f(t,t)$$  \hspace{1cm} (81)

where the last step follows from the fact that

$$\frac{d}{dt'} f(t',t) = b \wedge f(t',t).$$  \hspace{1cm} (82)

we have

$$b \wedge f(t,t) = (-\Delta, 0, \epsilon(t)) \wedge (0, 0, 1) = \Delta e_y$$  \hspace{1cm} (84)

so

$$e_z \wedge (b \wedge f(t,t)) = \Delta e_z \wedge e_y = -\Delta e_x.$$  \hspace{1cm} (85)

We thus find that the dissipation term (80) becomes:

$$\chi = \frac{\eta_0^2}{2\hbar} (-\Delta) e_x$$

$$= -\pi \alpha \Delta e_x$$

$$= \chi e_x$$  \hspace{1cm} (86)

We note that this term acts in the negative $e_x$ direction. By taking the dot product of $a$ with (75) to find $\partial^2 a / \partial t^2$ we see that the dissipation term thus tends to reduce the length of the vector $a$, in contrast to the magnitude-conserving spin precession term. This is directly analogous to the way that an electric field can change a speed while a magnetic field cannot, in the Lorenz force law.
B. Additional simplification of fluctuation term in zero temperature limit:

We have, provided that \( \omega_c \tau \gg 1 \),

\[
Q_2(v) = \frac{\eta}{\pi} \left[ \frac{\omega_c^2 - v^2}{(\omega_c^2 + v^2)^2} + \frac{1}{v^2} - \left( \frac{\tau}{\pi} \sinh \frac{\pi v}{\tau} \right)^{-2} \right]
\]  
(87)

This has two components corresponding to zero and finite temperatures respectively. We will here specialize to the zero temperature limit. In this case \( \psi_3 \) becomes \(-2\pi\alpha\) while \( \psi_x \) and \( \psi_y \) tend to zero.

V. APPLICATION TO LANDAU-ZENER-STUCKELEBERG PROBLEM:

The dissipative LZS problem as usually considered (e.g. [18]) corresponds to the driven spin-boson Hamiltonian with the specific choice \( \epsilon(t) = \epsilon t \), although other choices may be of interest (e.g. [22]). We emphasise that in this paper we have kept general time dependence \( \epsilon(t) \) of \( \mathbf{1} \) up to now. The standard LZS choice corresponds to a spin modelling a particle in a biased double potential well for which an external driving force acts to reverse the sign of the offset between the wells at \( t = 0 \); \( t \) having increased from a large negative starting value \( t = t_0 \). The quantities of interest are usually the long time, e.g. \( t \to \infty \), values of the probability \( P_{LZS} \) that the spin is in the "down" \((-1)\) orientation if started "up" (the conventional "tunnelling probability") or, equivalently, the long positive time expectation values \( a_x, a_y, a_z \) of the spin operator \( \sigma \).

In absence of coupling to environment the LZS tunnelling probability can be obtained exactly as (e.g. [22, 25]):

\[
P_{LZS} = 1 - e^{-\pi \Delta^2 / 2 \epsilon} = 1 - e^{-\pi \Delta \tau_z} \]  
(88)

where \( \tau_z = \Delta / \epsilon \) is the Zener (characteristic tunnelling) time.

\( P_{LZS} \) is \( \sim 1 - e^{-S / \hbar} \) where the action \( S \) is the energy for one hop times the Zener time, which, to within a numerical factor, can be derived from an instanton calculation [8]. The inverse of the tunnelling angular frequency expressed in units of \( \tau_z \) is \( 2 / (\Delta \tau_z) = \lambda \), a nonadiabaticity parameter [27], which increases as the speed of change of the energy levels increases i.e. as the system becomes more nonadiabatic.

Figures 1 and 2 illustrate the Landau-Zener behaviour (see also [25]). For large \( \lambda \) the value of \( S \) tends to zero, as does \( P_{LZS} \) and so the probability of not tunnelling tends to 1 i.e. in the fast passage limit the system does not tunnel. In the opposite limit of adiabatically slow change, the particle clings to the instantaneous eigenstate and must tunnel, so \( P_{LZS} \) tends to \( 1 \), i.e. the probability of not tunnelling tends to 0.

A. Illustrative numerical solutions of ohmic Bloch-Redfield equation at zero temperature

To solve our Bloch-Redfield equations we need to rescale time to the Zener time \( \tau_z \). After doing this the ohmic version becomes:

\[
\frac{\partial a}{\partial T} = B \wedge a(T) + \frac{2\pi \alpha}{\lambda} e_x - e_z \wedge (\psi(T) \wedge a(T)) \]  
(89)

We first note that this form shows why the effect of the dissipation term is negligible for the (fast passage) non-adiabatic limit of large \( \lambda \). It is simply because the dissipation term is inversely proportional to \( \lambda \). This means that (within the limits of our approximation) the faster a damped qubit is switched, the less it will be affected.

We show representative solutions of [50] in the absence of fluctuations as an illustration of the size of the perturbation of the probability caused by the spin-bath coupling. Figure 3 shows how \((1/2)(1 + a_z)\) changes in the most adiabatic case studied, \( \lambda = 1 \), comparing the uncoupled evolution (blue curve) with the fast passage case \( \lambda = 0.001 \). Figure 4 is for the same case as Figure 3 but shows the 3 components of spin, only for the damped case. Figures 5 and 6 are analogous but show the fast passage \( \lambda = 15 \) case. Figures 7 and 8 are also for the fast passage case \( \lambda = 15 \) but are for stronger coupling to the bath \( \alpha = 0.01 \). At this level of coupling the damping of quantum oscillations is very noticeable, although it does not alter the final tunnelling probability.

VI. CONCLUSIONS

This paper has extended the static spin boson study of Waxman [17] to the driven spin boson case, obtaining an exact integro-differential equation for the time evolution of the propagator of the reduced spin density matrix, the first main result. By specializing to weak damping we then obtained the next result, a set of Bloch-Redfield equations for the equilibrium fixed spin initial condition. Finally we showed that these equations can be used to solve the classic dissipative Landau-Zener problem and illustrated these solutions for the weak damping case. The effect of dissipation was seen to be minimised as passage speed increased, implying that qubits need to be switched as fast as possible.

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APPENDIX A: NOTATION

- \( \alpha \): dimensionless coupling constant
- \( a(t, t_0) \): spin polarisation vector
- \( a^{(0)}(t, t_0) = \equiv f(t, t_0) \): spin polarisation vector in uncoupled case
- \( A[\sigma] \): Spin amplitude functional for path containing \( n \) flips
- \( \hat{A}[\sigma, \hat{f}] \): Spin amplitude in stochastic case
- \( \beta \): Inverse temperature
- \( b \): vector derived from 2-level Hamiltonian
- \( \{c_\alpha\} \): Set of spin-bath coupling constants \( c_\alpha \)
- \( d[\hat{x}] \): measure for path integral
- \( d[\sigma] \): measure for spin path integral
- \( \Delta \): tunnelling matrix element
- \( D[\sigma] \): Correlation function in stochastic case
- \( \epsilon(t) \): bias
- \( \eta \): ohmic coupling strength
- \( f \): Fluctuating force
- \( F[\sigma, \nu] \): Influence functional
- \( F_{A=0} \): Influence functional in uncoupled case
- \( \hat{e}_x, \hat{e}_y, \hat{e}_z \): unit vectors
- \( h \): Planck constant
- \( H(t) \): Hamiltonian with corresponding action \( S[\sigma, x] \)
- \( H_0 \): Hamiltonian with corresponding action \( S_0[x] \)
- \( H_B(t) \): Bath Hamiltonian with corresponding action \( S_B[x] \)
- \( H_I(t) \): Interaction Hamiltonian with corresponding action \( S_I[\sigma, x] \)
- \( H_\Sigma(t) \): Spin Hamiltonian with corresponding action \( S_\Sigma[\sigma] \)
- \( J(\omega) \): bath spectral function
- \( K^{(0)}(t) \): spin propagator for \( \hat{\rho}^{(0)} \)
- \( K(t) \): spin propagator for \( \hat{\rho} \)
- \( \chi \): dissipation term
- \( k_B \): Boltzmann constant
- \( \lambda \): adiabaticity parameter
- \( m_\alpha \): oscillator mass
- \( \omega_\alpha \): oscillator frequency
- \( \omega_c \): bath cutoff
- \( \psi_i \): \( i = x, y, z \)
- \( P_LZS \): Landau-Zener tunnelling probability
- \( P[f] \): stochastic force probability functional
- \( q_0 \): inter-well spacing
- \( Q_1 \): retardation function
- \( Q_2 \): fluctuating force correlation function
- \( \rho_{osc} \): Single oscillator density matrix
- \( \rho \): density matrix
- \( \hat{\rho} \): spin density matrix
- \( \sigma_{x,y,z} \): Pauli spin matrices
- \( \tau_z \): Zener time
- \( t \): time
- \( t_0 \): fiducial time
- \( T \): temperature
- \( U \): unitary time evolution operator
- \( \{x_\alpha\} \) (or \( \mathbf{x} \)): set of harmonic oscillator positions \( x_\alpha \)
- \( Z_0 \): partition function
- \( z_1, z_2 \): temporary sum and difference co-ordinates

APPENDIX B: IDENTIFICATION OF FLUCTUATING FORCE AND DERIVATION OF STOCHASTIC EQUATION OF MOTION FOR PROPAGATOR OF DRIVEN SPIN-BOSON SYSTEM

We now show that the second term in the influence functional is equivalent to a random fluctuating force leading to an alternative equation of motion for the propagator of stochastic (quantum Fokker-Planck) type. This result is still quite general, but we confirm that the known delta-correlated force would be recovered in the high temperature limit for an ohmic choice of spectral density.

We first define a probability functional \( P[\hat{f}] \) which gives the probability that a member of a statistical ensemble experiences a force \( \hat{f} \) at a given instant:

\[
P[\hat{f}] = \exp\left(-\frac{1}{2} \int \hat{f}(u) D^{-1}(u, v) \hat{f}(v) \right) \tag{B1}
\]

normalised such that

\[
\int d[\hat{f}] P[\hat{f}] = <1> = 1. \tag{B2}
\]

Then we define an average over the ensemble of forces

\[
< e^{-\int \hat{f}(u) h(u)} >_f = e^{\frac{1}{2} \int h(u) D(u, v) h(v)} \tag{B3}
\]

which implies that the autocorrelation function is given by

\[
< \hat{f}(u) \hat{f}(v) >_f = D(u, v). \tag{B4}
\]

If we expand \( D(u, v) \) in terms of its eigenvalues \( \{\lambda_n\} \)

\[
D(u, v) = \sum_n \lambda_n \phi_n(u) \phi_n(v) \tag{B5}
\]

we can define its inverse \( D^{-1}(u, v) \) by

\[
D^{-1}(u, v) = \sum_n \lambda_n^{-1} \phi_n(u) \phi_n(v) \tag{B6}
\]

where we require \( \lambda_n > 0 \) for all \( n \). We define the correlation function \( Q_2(u, v) \) through

\[
D(u, v) = 2\hbar Q_2(u - v). \tag{B7}
\]

Hence if we take the average

\[
< e^{-\frac{1}{2} \int_{t_0}^t du [\sigma(u) - \nu(u)] \hat{f}(u)} >_f = e^{-\frac{1}{2} \left( \frac{2}{\beta} \right)^2 \int_{t_0}^t du \int_{t_0}^t dv [\sigma(u) - \sigma(v)] [\sigma(v) - \sigma(v)] Q_2(u - v)} \tag{B8}
\]
we obtain an object which has the same form as the second, real factor in the influence functional \( \tilde{Q}_2(u-v) \). The identification of the correlation function \( Q_2(u-v) \) can be made with our previously defined \( Q_2(u-v) \) provided that the Fourier transform is positive. We recall that \( Q_2 \) is of the form of a cosine transform so we can see positivity is satisfied.

We can thus define a new amplitude \( A[\sigma, \tilde{f}] \) and an influence functional \( \tilde{F}[\sigma, \nu] \) via

\[
A[\sigma, \tilde{f}] = (\frac{i\Delta}{2})^n \exp -\frac{i}{\hbar} \int_0^t du (\frac{\hbar \tilde{f}(u)}{2}) \sigma(u) \quad (B9)
\]

where we denoted the stochastic propagator by \( \tilde{K} \). This propagator equation could now be used with \( \tilde{K} \) to obtain a quantum Fokker-Planck equation for the driven spin-boson model, analogously with [17, 26].

The replacement of the \( Q_2 \) term has thus contributed a fluctuating bias to the existing time dependent bias. In consequence the stochastic analogue of the Bloch-Redfield equation [40], before averaging with respect to \( \tilde{f} \), becomes:

\[
\frac{\partial a}{\partial t} = b(t) \wedge a + \chi + \frac{q_0}{\hbar} \tilde{f}(t) \hat{e}_z \wedge a \quad (B12)
\]

This is a weak damping quantum Langevin equation. Here \( \langle \tilde{f}(u)\tilde{f}(v) \rangle = 2\hbar Q_2(u-v) \) and \( \langle a \rangle \) is the physical quantity. \( \tilde{f}(t) \) has the physically appealing interpretation of being the fluctuating force on the spin associated with a given member of the ensemble of systems considered. We believe that this may be more tractable than the Bloch-Redfield form in cases when the retarded integrals would otherwise need to be evaluated.

We note that we can recover the known delta-correlated behaviour of \( Q_2 \) for the high temperature \( (\tau \to 0) \), ohmic spectral density (Eq. 46) limit. Using [40] we first substitute for \( J(w) \) in \( \tilde{K} \), and then, provided the bath cutoff frequency \( \omega_c \) is sufficiently large but \( \omega_c^2 = \hbar \omega/k_B T \) still sufficiently small, we can approximate \( \coth x \) by \( 1/x \). This gives us \( Q_2 = \frac{2\hbar k_B T}{\pi \hbar} \delta(u) \) and thus

\[
\langle \tilde{f}(t)\tilde{f}(t') \rangle = \frac{4\eta k_B T}{\pi} \delta(t-t') \quad (B13)
\]

and

\[
\tilde{F}[\sigma, \nu] = \exp -\frac{i}{\hbar} \frac{q_0}{2} \int_0^t du \int_0^t dv [\sigma(u) - \sigma(v)] [\sigma(v) + \nu(v)] Q_2'(u-v) \quad (B10)
\]

The stochastic analogue of (17) is, before averaging with respect to \( \tilde{f} \):

\[
\begin{align*}
\hbar & \partial_t \tilde{K}(\sigma_1 \sigma_2 t | \sigma_3 \sigma_4) = -\frac{\hbar \Delta}{2} \tilde{K}(\sigma_1 \sigma_2 t | \sigma_3 \sigma_4) - \tilde{K}(\sigma_1 - \sigma_2 | \sigma_3 \sigma_4) \\
& \quad + \left( \frac{\hbar e(t)}{2} + \frac{q_0}{2} \tilde{f}(t) \right) (\sigma_1 - \sigma_2) \tilde{K}(\sigma_1 \sigma_2 t | \sigma_3 \sigma_4) \\
& \quad + \left( \frac{q_0}{2} \right)^2 (\sigma_1 - \sigma_2) \int_0^t dv Q_2'(t-v) < \sigma(v) + \nu(v) >,
\end{align*}
\]

APPENDIX C: GREEN’S FUNCTION SOLUTION OF OHMIC QUANTUM LANGEVIN EQUATION

We here solve the quantum Langevin equation perturbatively using the Green function method of Zhang [17]. We find the intriguing result in the ohmic weak damping case that the fluctuations enter only at second order in \( \alpha \), and so give an expression for the tunnelling probability to first order in \( \alpha \).

We use the methods of equations (46-52) of [17], but unlike Zhang we do not differentiate the Green’s function solution.

We have:

\[
\frac{\partial a}{\partial t} = b(t) \wedge a + \chi + \frac{q_0}{\hbar} \tilde{f}(t) \hat{e}_z \wedge a \quad (C1)
\]

where \( \tilde{f}(t) \) is the fluctuating force. This allows us to write a solution of the stochastic equation as

\[
a(t, \tilde{f}) = M(t, t_0) a(t_0) + \int_{t_0}^t M(t, t') \chi(t') dt' \quad (C2)
\]

(c.f. equation (46) of [17]) with \( M \) a Green function for the homogeneous equation

\[
\frac{\partial a}{\partial t} \wedge b + \chi \wedge a - \frac{q_0}{\hbar} \tilde{f}(t) \hat{e}_z \wedge a = 0 \quad (C3)
\]

We then take out the evolution operator \( u(t, t') \) for the unperturbed spin, and then (equation (49) of [17] rearranged) note that

\[
u(t, t') N(t, t') = M(t, t') \quad (C4)
\]
\[ a(t, f) = u(t, t_0)N(t, t_0) + \int_{t_0}^{t} u(t, t') N(t, t') \chi(t') dt'. \]  
(C5)

Now, following equation (52) of [17], the formal solution for \( N \) is

\[ N(t, t') = 1 + \sum \int_{t'}^{t} dt_1 \ldots \int_{t'}^{t_n-1} dt_n \mathcal{F}(t_1, t') \mathcal{F}(t_n, t') \]  
(C6)

\[ a(t) = \langle a(t, \tilde{f}) \rangle = u(t, t_0) < N(t, t_0) > a(t_0) + \int_{t_0}^{t} u(t, t') < N(t, t') > \chi(t') dt' \]  
(C8)

Now \(< N(t, t_0) > \) is

\[ 1 + \int_{t_0}^{t} dt_1 < \mathcal{F}(t_1, t') > + \int_{t_0}^{t} \int_{t_0}^{t_1} dt_1 dt_2 < \mathcal{F}(t_1, t') \mathcal{F}(t_2, t') > \]  
(C9)

fluctuating force without serious loss of generality. We note that

\[ < N(t, t_0) > a(t_0) = \left[ 1 + \int_{t_0}^{t} \int_{t_0}^{t_1} dt_1 dt_2 < \mathcal{F}(t_1, t') \mathcal{F}(t_2, t') > \right] a(t_0) \]  
(C10)

\[ = \left[ 1 + \frac{q_0^2}{\hbar^2} \int_{t_0}^{t} \int_{t_0}^{t_1} dt_1 dt_2 < \tilde{f}(t_1) \tilde{f}(t_2) > \hat{e}_z \wedge (\hat{e}_z \wedge) a(t_0) \right] a(t_0) \]  
(C11)

because [\( \hat{e}_z \wedge (\hat{e}_z \wedge) a(t_0) = 0 \) for the case we chose, where \( a(t_0) \) was \( (0, 0, 1) \). The terms under the Green’s function integral (i.e. equation (C8) for \( N(t, t') \chi(t') \) are all second order in \( \alpha \) except the first one which from above expansion can be seen to be just \( \chi(t') \), so we are left with a very simple solution

\[ a(t) = u(t, t_0) a(t_0) + \int_{t_0}^{t} u(t, t') \chi(t') dt'. \]  
(C12)

\[ = a^0(t, t_0) + \chi \int_{t_0}^{t} a^{(1)(0)}(t, t') dt' \]  
(C13)

where \( a^{(1)(0)}(t, t') \) is just the undamped solution \( a^0 \) at time \( t \), but started at \( (1, 0, 0) \) at \( t' \). In the ohmic case after rescaling times by \( \tau_2 \) we have \( \chi = 2\pi\alpha/\lambda \) (c.f. [89]) so we have a linear dependence on \( \alpha \) for a given \( \lambda \). Checking this prediction with numerical solutions for \( \alpha = 0.005 \) agrees very well with the above result. We note this is a consequence of the spin-up initial condition, as others might give a first order contribution from the fluctuating force. It is however independent of the spectral form of the environment once that initial condition has been specified.
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FIG. 1: Dependence of the Landau-Zener-Stuckelberg tunnelling probability $P_{LZS}$ and the probability of not tunnelling $1 - P_{LZS}$ on the adiabaticity parameter $\lambda$ in the absence of spin-bath coupling.
FIG. 2: Evolution from $t = -10\tau_z$ of $1 - P_{LS}$ to $t = 10\tau_z$ for spins started with $\mathbf{a} = (0, 0, 1)$ in the absence of spin-bath coupling (after Berry [25]). $\lambda$ increases as the curves go up the plot, taking values of 1, 2.5, 5, 15.
FIG. 3: The evolution of $(1/2)(1 + a_z)$ with time in medium passage case, $\lambda = 1$, comparing the uncoupled evolution (blue curve) with $\alpha = 0.001$ (red curve).
FIG. 4: Three components of spin for the same case as Figure 3 showing only the damped cases.
FIG. 5: As Figure 3 but for the fast passage case $\lambda = 15$. 

Zero temperature: fast passage: $P_+^{\alpha=0.001 \lambda=15}$
Zero temperature: $\alpha=0.001 \lambda=15$: Components of damped a vector

FIG. 6: As Figure 4 but for the fast passage case $\lambda = 15$. 
FIG. 7: As Figure 5 but for stronger coupling to the bath $\alpha = 0.01$. At this level of coupling the damping of quantum oscillations is very noticeable, although it does not alter the final tunnelling probability.
Zero temperature: $\alpha=0.01 \, \lambda=15$: Components of damped a vector

FIG. 8: As Figure 6 but for stronger coupling to the bath $\alpha = 0.01$. 