Single Electron Spin in Interacting Nuclear Spin Bath — Coherence Loss and Restoration

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Issues and Problems

• Single spin in solids: decoherence and coherence protection

Single electrons localized in solids



Issues and Problems

- Single spin in solids: decoherence and coherence protection
- A 2-level system + many interacting bath spins

Theory of the spin bath

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Abstract

The quantum dynamics of mesoscopic or macroscopic systems is always complicated by their coupling to many 'environmental' modes. At low *T* these environmental effects are dominated by *localized* modes, such as nuclear and paramagnetic spins, and defects (which also dominate the entropy and specific heat). This environment, at low energies, maps onto a 'spin bath' model. This contrasts with 'oscillator bath' models (originated by Feynman and Vernon) which describe *delocalized* environmental modes such as electrons, phonons, photons, magnons, etc. The couplings to *N* spin bath modes are *independent* of *N* (rather than the $\sim O(1/\sqrt{N})$ dependence typical of oscillator baths), and often strong. One cannot in general map a spin bath to an oscillator bath (or vice versa); they constitute distinct 'universality classes' of quantum environment.

Theories antecedent on spin bath

Spectral diffusion theory

- Herzog & Hahn, PR 56", Klauder & Anderson, PR 61", semi-classical theory

Electron nuclear hyperfine interation

- Schulten & Wolynes, J. Chem. Phys., 78" -frozen nuclear configuration
- Merkulov, Efros & Rosen, PRB 02"
- Khaetskii, Loss & Glazman, PRL 02", Coish & Loss, PRB 04"
- Schliemann, Khaetskii & Loss, PRB 02" sys-bath entanglement
- Shenvi, De Sousa & Whaley, PRB 05" small environment ~10 nuclei

Nuclear dipolar interaction plus diagonal e-n hyperfine coupling

- De Sousa & Das Sarma, PRB 03" semiclassical stochastic solution
- De Sousa, Shenvi & Whaley, PRB 05" -semiclassical theory
- Witzel, De Sousa & Das Sarma, PRB 05" ensemble study

Other low energy modes mapped to spin bath

- Prokov'ef & Stamp, Rep. Prog. Phys. 00" - magnets and superconducting systems

Sorry, not an exhaustive list.

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- Single spin in solids: decoherence and coherence protection
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- Single electron in III-V semiconductor quantum dot

Spin decoherence in QD: Phonon Vs. Nuclei

Decoherence by phonon scattering

• Spin relaxation $T_1 \sim ms - s$, at $\sim K$ in QD

theories (Khaetskii and Nazarov; Woods, Reinecke and Lyanda-Gella); experiments (Tarucha group; Kouwenhoven group; Finley group; Steel group)

 Pure dephasing suppressed at low-temp theoretical estimation: T₂ = 2T₁ @ ~ K and below (Golovach, Khaestskii and Loss, PRL 04'; Semenov & Kim, PRL 04')

<u>Spin transverse decoherence time from exp</u>

- Single spin T_2 ? not measurable with current capability
- $T_2^* \sim 1-10$ ns $\rightarrow T_1$ gated dot in GaAs, SAD
- $T_{H} \sim 1.2 \ \mu s \gg T_{1}$ gated dot in GaAs (Petta ea., Koppens ea.)

<u>Nuclear spin is the dominant cause for transverse</u> <u>decoherence at low temp.</u>

Electron spin in a nuclear spin bath



E-N coupled through contact hyperfine interaction
 Mesoscopic size N ~ 10⁶, posterior justification

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Electron nuclear dynamics



Issues and Problems

- Single spin in solids: decoherence and coherence protection
- A 2-level system + many interacting bath spins
- Single electron in III-V semiconductor quantum dot
 - Low T and high field
 - Pure transverse decoherence $(T_1 \rightarrow \infty)$
 - Mescoscopic nuclear bath, N ~ 10⁶, unpolarized
 - 1 + N well isolated from the rest universe
- Quantum mechanical origin of decoherence: entanglement

Decoherence of single quantum system



- Bath dynamics conditioned on system states
- Bath state bifurcates in the Hilbert space
- System (which-state) information measured by the bath
- Decoherence: decays of off-diagonal DM element (T₂) Nuclear correlation func: $\mathcal{L}_{+,-}^{s}(t) \equiv \langle J^{-}(t) | J^{+}(t) \rangle$; $\rho_{+,-}^{e}(t) = \mathcal{L}_{+,-}^{s}(t)\rho_{+,-}^{e}(0)$

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- Coherence restoration by disentanglement

Recoherence by disentanglement



- Flip of system states redirects bath evolution
- Bath states intersect in Hilbert space (which-state info erased)
- System disentangled from bath \rightarrow Coherence restored
- Possible in mesoscopic bath: sys+bath isolate from rest universe

Nuclear spin dynamics: pair wise flip-flop

Elementary excitation:





Nuclear spin dynamics: pair wise flip-flop

- Unconnected pair-flips are independent

$$|J\rangle \equiv |j_1\rangle \cdots |j_k\rangle \cdots |j_l\rangle \cdots |j_m\rangle \cdots |j_n\rangle \cdots |j_N\rangle$$
Unconnected
$$|j_k + 1\rangle \cdots |j_l - 1\rangle |j_m - 1\rangle \cdots |j_n + 1\rangle$$

$$|j_l - 2\rangle \cdots |j_m + 1\rangle$$

- Number of nuclear available for flip large ~ N (~10⁶) for typical $\left|J\right\rangle$
- Number of flips much smaller than N

$$N_{\text{flip}} = \sum_{k_1} \left| C_{J,k_1} \right|^2 + 2 \sum_{k_1,k_2} \left| C_{J,k_1,k_2} \right|^2 + 3 \sum_{k_1,k_2,k_3} \left| C_{J,k_1,k_2,k_3} \right|^2 + \dots \qquad N$$

- Probability of having connected pair-flips

$$P_{\rm con} \approx 1 - \exp\left(-N_{\rm flip}^2/N\right) = 1$$

Pair-Correlation-Method

 The two states connected by n-n pair-flip interactions is mapped into one two-state system (kth pseudo-spin).

Flip-pair to pseudo spin:
$$|j_n\rangle|j_m\rangle \Rightarrow |\uparrow\rangle_k$$
, $|j_n+1\rangle|j_m-1\rangle \Rightarrow |\downarrow\rangle_k$ flip-flop of nuclear pair mapped to single pseudo spin flipInitial state: $|J\rangle \Rightarrow \bigotimes_k |\uparrow\rangle_k$

- The dynamics of the pseudo-spins (pair-flips) is treated independent of each other.

Flip-flop dynamics to
pseudo spin rotations: $|J^{\pm}(t)\rangle \Rightarrow \bigotimes_{k} |\psi_{k}^{\pm}\rangle, \quad |\psi_{k}^{\pm}\rangle \equiv e^{-i\mathcal{H}_{k}^{\pm}t} |\uparrow\rangle_{k}$ Nuclear correlation func: $\mathcal{L}_{t,-}^{\epsilon}(t) = |\langle J^{-}(t) | J^{+}(t) \rangle| = \prod_{k} |\langle \psi_{k}^{-}(t) | \psi_{k}^{+}(t) \rangle|$

WY, Liu and Sham, PRB 74, 195301, 2006

Pair-Correlation-Method

- Verified from a linked cluster expansion approach.



Independent pseudospin rotations:

$$e^{\Box} = 1 + \Box + (1/2!) \Box \Box \Box + \dots$$

Saikin, WY and Sham, PRB 75, 125314, 2007

Geometrical picture for decoherence

 $\mathbf{h}_{k}^{\pm} = \left(B_{k} \pm A_{k}, 0, D_{k} \pm E_{k}\right) \qquad i\partial_{t} \left|\psi_{k}^{\pm}(t)\right\rangle = \left(\mathbf{h}_{k}^{\pm} \cdot \hat{\mathbf{0}}_{k}/2\right) \left|\psi_{k}^{\pm}(t)\right\rangle$

- Rotation of Bloch vector $S_k^{\pm} = \langle \psi_k^{\pm}(t) | \mathbf{\hat{o}}_k | \psi_k^{\pm}(t) \rangle$ in effective field \mathbf{h}_k^{\pm} .
- Distance $\delta_k = |S_k^+ S_k^-| = \sqrt{1 |\langle \psi_k^-(t) | \psi_k^+(t) \rangle|^2}$ is a direct measure of electron spin coherence.





Two mechanisms for pair-flip

Step 1: sort out all pseudo-spins (flip-pairs) from a given configuration $\mathcal{L}_{t,-}^{s}(t) = \left| \left\langle J^{-}(t) \middle| J^{+}(t) \right\rangle \right| = \prod_{k} \left| \left\langle \psi_{k}^{-}(t) \middle| \psi_{k}^{+}(t) \right\rangle \right|$

Step 2: determine the pseudo-field from 1st-principle interactions

$$\mathbf{h}_{k}^{\pm} = \left(B_{k} \pm A_{k}, 0, D_{k} \pm E_{k}\right) \qquad i\partial_{t} \left|\psi_{k}^{\pm}(t)\right\rangle = \left(\mathbf{h}_{k}^{\pm} \cdot \hat{\mathbf{0}}_{k}/2\right) \left|\psi_{k}^{\pm}(t)\right\rangle$$

 D_k by diagonal nuclear couplings Non-local pairs: Extl^{Q2}s⁻¹ n-n interaction dominant

 $\mathbf{h}_{k}^{E} = \underbrace{\pm}_{A_{k}}^{A}, 0, \pm E_{k}^{A}$

Local pairs: Intrinsic hyperfine mediated nuclear coupling infinite-range, $\propto B^{-1}$, $1-10 \text{ s}^{-1}$ (for $B \sim 40-1 \text{ T}$) $\mathbf{h}_{k}^{\pm} = \begin{pmatrix} B_{k}, 0, \pm E_{k} \end{pmatrix} \qquad \sim \text{N pairs, no field dependence}$ $B_{k}^{\pm} \text{ intrinsic nuclear coupling}$ finite-range, 10^{2} s^{-1} for near neighbors



Presented at the PITP/SpinAps Asilomar Conference in June 2007

Single spin FID: intrinsic vs extrinsic

Nuclear bath begins on a pure state of random configuration



Single System FID: field dependence

Nuclear bath begins on a pure state of random configuration



Ensemble dynamics

Single system (t=0):
$$|\psi^e(0)\rangle \otimes |J\rangle$$
Ensemble (t=0): $\rho(0) = \rho^e(0) \otimes \sum_J P_J |J\rangle \langle J|$ Ensemble correlation function:nuclear Overhauser
field $\mathcal{E}_J = \sum_n a_n j_n$ by the spectrum of
flip-pairs of $|J\rangle$ $\rho_{+,-}^e(t) = \mathcal{L}_{+,-}^{en}(t)\rho_{+,-}^e(0)$ $\mathcal{L}_{+,-}^{en}(t) = \sum_J P_J e^{-i\mathcal{E}_J t} |\langle J^-(t) | J^+(t) \rangle|$

- Number of flip-pairs $M \sim N$ (or N^2) for most $|J\rangle$
- Identical excitation spectrum up to an error of
- Identical temporal behavior for $\left|\left\langle J^{-}(t) \right| J^{+}(t) \right\rangle$

$$- \mathcal{L}_{+,-}^{en}(t) = \left| \left\langle J_0^{-}(t) \middle| J_0^{+}(t) \right\rangle \right| \sum_{J} P_J e^{-i\mathcal{E}_J t}$$

System-bath entanglement

Inhomogeneous broadening $\sum_{J} P_{J} e^{-i\mathcal{E}_{J}t} = e^{-(t/T_{2}^{*})^{2}}, T_{2}^{*} \sim 10 \text{ ns}$

 $1/\sqrt{M}$

Single System FID and Ensemble Echo

Nuclear bath begins on a pure state of random configuration



WY, Liu and Sham, PRB 74, 195301, 2006

Ensemble Spin Echo



Decoherence due to hyperfine mediated nuclear interactions is removed in spin echo!

(also in simulation with ~10 bath spin, Shenvi, deSousa and Whaley, PRB 05")



Spin echo measures the single spin decoherence induced by intrinsic nuclear interactions only ! $T_{H} = \sqrt{2}T_{2R}$



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Control of Bath Evolution for Disentanglement





- Flip of electron redirects evolution of bath
- Pseudo-spin paths re-intersects
- Universally at $\sqrt{2}\tau\,$ for all pseudospins
 - System disentangled from bath $(\alpha |+\rangle + \beta |-\rangle) \otimes |J(\sqrt{2}\tau)\rangle$

WY, Liu and Sham, PRL 98, 077602, 2007 Liu, WY and Sham, cond-mat/0703690

Coherence Echo in Single System Dynamics

Nuclear bath begins on a pure state of random configuration

 $d = 6 \text{ nm}, r_0 = 40 \text{ nm}, B = 10 \text{ T}, \text{ intrinsic n-n interaction dominant}$



- Different from dynamical decoupling, sys-bath coupling does not vanish

$$e^{-iH_{\rm eff}\sqrt{2}\tau} \equiv e^{iH^{-}(\sqrt{2}-1)\tau}e^{-iH^{+}\tau} \Longrightarrow H_{\rm eff} \neq 0$$

Disentanglement Concealed in Ensemble Dynamics

 $d = 6 \text{ nm}, r_0 = 40 \text{ nm}, B = 10 \text{ T}, \text{ intrinsic n-n interaction dominant}$



Disentanglement Concealed in Ensemble Dynamics

To observe quantum disentanglement in ensemble dynamics

a. Filter inhomogeneous broadening by measurement projection

Schemes to be realized in near future:

Klauser, Coish & Loss, PRB 2006

Giedke, Taylor, D'Alessandro, Lukin & Imamoglu, PRA 2006

Stepanenko, Burkard, Giedke & Imamoglu, PRL 2006

or

b. Arrange disentanglement time to coincide ensemble echo time

WY, Liu and Sham, PRL 98, 077602, 2007 Liu, WY and Sham, cond-mat/0703690

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Two-pulse control: Disentanglement at echo time



Concatenated Dynamical Disentanglement

Concept of concatenation on dynamical decoupling, Khodjasteh and Lidar, PRL 05"



- Disentanglement occur at $\tau_l = 2^l \tau$
- Decoherence reduced by $\left(b au_l
 ight)^2$ with each level of concatenation
- Controlling small parameter: bath spin interaction $b = 10^2 s^{-1}$

Concatenated Dynamical Disentanglement

$$\exp\left(-t^{2l+2}/T_{c,l}^{2l+2}\right)$$



WY, Liu and Sham, PRL 98, 077602, 2007 Liu, WY and Sham, cond-mat/0703690





Stabilization with repeated # of Concatenated units

Summary

✓ 1+N isolated from rest universe in relevant timescale

 Quantum theory of decoherence: bath evolution conditioned on system state

- Decoherence by sys-bath entanglement
- Operations on system affects bath evolution
- Spin echo removes more than inhomogenesous dephasing
- Echo decay time T_H NOT equivalent to single spin T_2
- ✓ Slow bath dynamics: pair-correlations dominates
- Sys-bath disentanglement by pulse sequences on electrontenation design more efficient then periodic sequence.



Canonical transformation:

$$\hat{W} \equiv \exp\left(\sum_{n} \frac{a_n}{2(\Omega_e - \omega_n)} (\hat{S}_e^+ \hat{J}_n^- - \hat{S}_e^- \hat{J}_n^+)\right)$$

Effective Hamiltonian:

$$\hat{H}_{red} = \hat{W}\hat{H}\hat{W}^{-1}$$

Rotation of wavefunction:

$$\hat{W}|\pm\rangle\otimes|\mathcal{J}\rangle\approx\left(1-\frac{1}{2}\sum_{n}|w_{n}^{\pm}|^{2}\right)|\pm\rangle\otimes|\mathcal{J}\rangle\mp\sum_{n}w_{n}^{\pm}|\mp\rangle\otimes|j_{n}\pm1\rangle\bigotimes_{m\neq n}|j_{m}\rangle$$

Visibility loss: $(\Omega_e \sqrt{N}/\mathcal{A})^{-2}\!\ll\! 1\,$ for B > 1T

Effective dynamics: $e^{-i\hat{H}t}|\pm\rangle\otimes|\mathcal{J}\rangle\cong e^{-i\hat{H}_{\mathrm{red}}t}|\pm\rangle\otimes|\mathcal{J}\rangle$

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Description of 2 level quantum system

Single quantum system

$$|\varphi\rangle = \alpha |+\rangle + \beta |-\rangle \qquad \rho \equiv |\varphi\rangle\langle\varphi| = \begin{bmatrix} |\alpha|^2 & \alpha\beta^* \\ \alpha^*\beta & |\beta|^2 \end{bmatrix}$$

Ensemble of identical quantum systems

$$\rho = \sum_{i=1}^{N} P_i |\varphi_i\rangle \langle \varphi_i | = \begin{bmatrix} \sum_{i}^{N} P_i |\alpha_i|^2 & \sum_{i}^{N} P_i \alpha_i \beta_i^* \\ \sum_{i}^{N} P_i \alpha_i^* \beta_i & \sum_{i}^{N} P_i |\beta_i|^2 \end{bmatrix}$$

Reduced density matrix for open quantum system

$$|\psi_{tot}\rangle = \sum_{i} |\alpha_{i}\rangle_{sys} \otimes |\beta_{i}\rangle_{en} \quad \Box \rangle \quad \rho_{sys} = Tr_{en}[|\psi_{tot}\rangle\langle\psi_{tot}|]$$

Decoherence: relaxation and pure dephasing

Geometric representation

$$\rho = \frac{1}{2}(I + \vec{a} \cdot \vec{\sigma}),$$

Bloch vector :

$$\frac{1}{2}\vec{a} = Tr\left[\rho\vec{S}\right]$$

 $a_{r} = 2 \operatorname{Re} \rho_{21}$ $a_{v} = 2 \operatorname{Im} \rho_{21}$ $a_{z} = \rho_{11} - \rho_{22}$



Longitudinal relaxation

 $T_2^{rl} = 2T_1$ Decay of coherence as a result of decay of population

Pure dephasing

 T_2^{deph}

No decay of population. Usually much faster than T_1



Inhomogeneous broadening & spin echo

