## Overview

- General concepts
- Bulk samples and devices with diffusive metallic transport
  - Quantum contributions to diffusive transport weak localization
  - Mechanisms of decoherence
  - Spin effects
- Mesoscopic devices
  - Coherent properties of qubits

# Aim: additional theoretical aspects relevant to the lecture by Dr. Oleg Astafiev

## Devices for quantum computation

- General
- Examples of implementation based on semiconductors and superconductors
  - -Josephson qubits

(see the lecture by Dr. O. Astafiev)

- Spin dynamics of qubits
- Mechanisms of decoherence brief discussion of the theoretical approaches.

#### What is the qubit from theoretical point of view?

Qubit is a typical quantum two-level system equivalent to ½ spin

The qubit is described by effective Hamiltonian

$${\cal H}_{
m ctrl} = -rac{1}{2}B_z \hat{\sigma}_z - rac{1}{2}B_x \hat{\sigma}_x \; .$$

with tunable  $B_x$  and  $B_z$  to perform single-qubit operations.

A controllable interaction in the form

$${\cal H}_{
m ctrl}(t) = -rac{1}{2}\sum\limits_{i=1}^N B^i(t) \hat{\sigma}^i + \sum\limits_{i
eq j} J^{ij}_{ab}(t) \hat{\sigma}^i_a \hat{\sigma}^j_b \ ,$$

(where a summation over spin indices a,b=x,y,z is implied) to

perform two-bit operations.



Spin dynamics is governed by the equation of motion for the spin operator

$$\dot{\boldsymbol{\sigma}} = rac{\imath}{\hbar} [\mathcal{H}, \boldsymbol{\sigma}]$$

Static magnetic field:  $\mathcal{H}_0 = -\frac{h\omega_0}{2}\sigma_z$ ,  $\omega_0 = \gamma B_0$ 

Spin algebra:  $\sigma_y \sigma_z = i \sigma_x$ ,  $\sigma_z \sigma_x = i \sigma_y$ ,  $\sigma_x \sigma_y = i \sigma_z$  $\sigma_i \sigma_k + \sigma_k \sigma_i = 2\delta_{ik}$ 

$$\delta = \omega_0 t$$

Precession around z-axis



Rotating magnetic field:

$$B_{x}(t) = B_{1} \cos(\omega_{e}t + \phi),$$
  

$$B_{y}(t) = B_{1} \sin(\omega_{e}t + \phi)$$
  

$$\mathcal{H}_{1} = -\frac{\hbar\omega_{1}}{2} \left[\sigma_{x} \cos(\omega_{e}t + \phi) - \sigma_{y} \sin(\omega_{e}t + \phi)\right], \quad \overset{\text{Rabi}}{\underset{\omega_{1}}{\text{frequency}}}$$

The rotating coordinate frame is defined as

$$|\chi\rangle_r = e^{-i\sigma_z\omega_e t/2}|\chi\rangle$$

$$\mathcal{H}_r = \frac{\hbar(\omega_0 - \omega_e)}{2} \sigma_z + \frac{\hbar\omega_1}{2} \left[\sigma_x \cos\phi - \sigma_y \sin\phi\right]$$

At  $\omega_0 = \omega_e$  - rotation around the axis in the xy-plane







Nutation with Rabi frequency The same motion in real space If the spin is detuned from the resonance the precession takes place around the tilted axis with  $\alpha = \arctan(\omega_1/\Delta\omega),$   $\Delta\omega \equiv \omega_0 - \omega_e,$  $\omega'_1 = \sqrt{\omega_1^2 + (\Delta\omega)^2}$ 



Precession part of magnetization is like having a magnet rotating around at very high speed (at AC frequencies)

It will generate an oscillating voltage in a coil of wires placed around the subject — this is magnetic induction. It decays due to relaxation.

A way to study precession and decoherence – Ramsey interference

## Ramsey interference





The projection to z-axis periodically depends on the distance between two pulses – Ramsey fringes

# Q: Can one measure decoherence by studying decay of the free induction oscillations?

A: Measurements of free induction is not very good to find spin properties.

If there are few close eigen frequencies, then the signal consists of beatings.



#### A way to avoid beatings: Refocusing methods

## Hahn spin echo

#### **Refocusing:**





Beatings are removed! Only true decoherence is left.

#### A way to describe mixed states – density matrix

For a pure state:  $\hat{\rho} \equiv |\chi\rangle\langle\chi| = \begin{pmatrix} |\chi_1|^2 & \chi_1\chi_2^* \\ \chi_2\chi_1^* & |\chi_2|^2 \end{pmatrix}$ 

$$\widehat{\rho} = \begin{pmatrix} \cos^2 \theta / 2 \leftarrow (1/2)e^{-i\delta}\sin \theta \\ (1/2)e^{i\delta}\sin \theta & \sin^2 \theta / 2 \end{pmatrix} \text{ probabilities}$$
angle

In general, for a mixture of different spin states:

$$\rho = \sum_{i} W_{i} |\chi_{i}\rangle \langle \chi_{i}|, \ \sum_{i} W_{i} = 1$$
  
 $W_{i}$  are partial probabilities

Expression through polarization:

$$\rho = \frac{1}{2} \begin{pmatrix} 1 + \mathcal{P}_z & \mathcal{P}_x - i\mathcal{P}_y \\ \mathcal{P}_x + i\mathcal{P}_y & 1 - \mathcal{P}_z \end{pmatrix}$$

I dentification pure states:

$$\operatorname{Tr} \rho^2 = \frac{1}{2} \left( 1 + |\mathcal{P}|^2 \right) \rightarrow 1$$

Decoherence is just decay of the polarization of effective spin.

Diagonal elements represent the energy decay, while off-diagonal – decay of coherent precession (true decoherence). Decay of diagonal elements means relaxation of the population of the spin states and, consequently, energy relaxation.

The characteristic time is denoted as  $T_1$ .

Off-diagonal elements describe spin precession. Their decay, allowed for by some relaxation time,  $T_{2'}$  is called decoherence, or dephasing.

I nelastic processes contribute to both energy relaxation and decoherence.

For a single inelastic relaxation process  $T_2=2T_1$ .

#### How one can make ½ spin from a macroscopic system?

#### Some examples based on semiconductors

The Loss-DiVinchenzo proposal, 1998 – controlling spins of the electrons localized in quantum dots



Zeeman splitting is produced by magnetic field created by the current. The coupling is controlled by the back gates modulating g-factor. The exchange interaction is controlled by front gates.

It is demonstrated (also experimentally) that the quantum operations can be performed by proper manipulations of the magnetic field and gate voltages.

(see Burkard, cond-mat/0409626, for a review of solid state devices)

#### **Charge-Qubit Operation of an Isolated Double Quantum Dot**

J. Gorman,<sup>1</sup> D. G. Hasko,<sup>1</sup> and D. A. Williams<sup>2</sup>



NTT BRL School, 2005

0

 $T_r$ 

A very promising way - using intrinsically coherent macroscopic systems – superconductors.

(details are given in the lecture by Dr. O. Astafiev, see also additional presentation)





#### The echo signal decays because of decoherence





The model is based on the account of charge hopping between traps and parts of the qubit. The calculations are based on the analysis of the qubit's density matrix





Proper choice of the working point can significantly decrease the coherence.

There are several beautiful implementations of this idea.

Theoretical approaches to decoherence

Quantum mechanics does not allow a phenomenological dissipation – a microscopic model is necessary

#### Spin-boson model

(Caldeira-Leggett)

assumption that the qubit interacts with a set of equilibrium bosons (phonons, electron-hole pairs, etc)

Does not properly describe the decoherence by low-frequency noise.

#### Model of dynamic disorder

assumption that the qubit interacts with a set of dynamic defects with broad distribution of relaxation rates, which produce low-frequency noise.

#### Spin-boson model:

$$\mathcal{H}_{0} = \frac{E}{2} (\cos \theta \, \sigma_{z} + \sin \theta \, \sigma_{x})$$

$$E = \sqrt{B_{z}^{2} + B_{x}^{2}}, \, \sin \theta \equiv B_{x}/E;$$

$$\mathcal{H}_{\text{int}} = \sigma_{z} \hat{\mathcal{X}}, \quad \hat{\mathcal{X}} = \sum_{j} C_{j} (\hat{b}_{j} + \hat{b}_{j}^{\dagger})$$

$$\frac{1}{2} - \text{spin interacting with a boson field}$$

$$\begin{array}{ll} \mathcal{H}_{0} & \rightarrow & \frac{E}{2}\sigma_{z} & & \text{Diagonalizing } \mathcal{H}_{0} \\ \mathcal{H}_{\text{int}} & \rightarrow & (\cos\theta \, \sigma_{z} - \sin\theta \, \sigma_{x}) \hat{\mathcal{X}} \\ & & \text{Shaking of levels} & & \text{Inter-level transitions} \end{array}$$

Decoherence is expressed through noise spectrum

$$S_{\mathcal{X}}(\omega) \equiv \left\langle \left[ \hat{\mathcal{X}}(t), \hat{\mathcal{X}}(0) \right]_{+} \right\rangle_{\omega} = 2J(\omega) \operatorname{coth} \frac{\omega}{2T}$$

 $J(\omega)\equiv\pi\sum_j C_j^2\,\delta(\omega-\omega_j)$  - bath spectral density

We need 
$$\langle e^{-i\Phi(t)} \rangle \rightarrow \operatorname{Tr} \left( e^{-i\widehat{\Phi}(t)} e^{i\widehat{\Phi}(0)} \widehat{\rho}_{bath} \right)$$
  
Environment-  
induced phase  $\hat{\Phi}(t) \equiv i \sum (2C_j/\omega_j) e^{i\mathcal{H}_b t} \left( \hat{b}_j^{\dagger} - \hat{b}_j \right) e^{-i\mathcal{H}_b t}$ 

j

fluctuation

Result for 
$$\mathcal{K}(t) = -\ln \operatorname{Tr} \left( e^{-i\hat{\Phi}(t)} e^{i\hat{\Phi}(0)} \hat{\rho}_b \right)$$
  
 $\mathcal{K}(t) = \frac{8}{\pi} \int_0^\infty \frac{d\omega J(\omega)}{\omega^2} \left[ \sin^2 \frac{\omega t}{2} \coth \frac{\omega}{2T} + \frac{i}{2} \sin \omega t \right]$ 

Derivation is based on the Gaussian assumption:  $\langle e^{i\varphi}\rangle = e^{-\langle \varphi^2\rangle/2}$ 

Result

$$1/T_{1} = \hbar^{-2} \sin^{2} \theta S_{\mathcal{X}}(E/\hbar)$$

$$1/T_{2} = 1/2T_{1} + \hbar^{-2} \cos^{2} \theta S_{\mathcal{X}}(0)$$
Direct transitions Shaking

Sources and types of noise will be discussed in the lectures by Profs. L. Levitov and C. Glattli.

The spin-boson model is not applicable to the decoherence by the low-frequency noise with spectrum  $S_{\mathcal{X}} \propto 1/\omega$ - the expression for decoherence is divergent.

It is based on the Gaussian assumption, which is not applicable to the 1/f-noise.

- 1/f noise is produced by parts of environment with long relaxation times – it is in general not a stationary Markov process;
- Long-range interactions between the qubit and fluctuating entities (fluctuators) lead to non-Gaussian effects

We will consider a simple solvable model, allowing for both effects – model of fluctuating charges

Paladino et al., 2002

Qubit is surrounded by *fluctuators*, which behave as twolevel systems. Example: charge traps near the gate.

The fluctuators randomly *switch between their states* due to interaction with phonons or electrons.

Decoherence is due to *time dependence* of the random fields, produced by the fluctuators.



Model and Theoretical MachineryHamiltonian: $\mathcal{H} = \mathcal{H}_q + \mathcal{H}_{man} + \mathcal{H}_{qF} + \mathcal{H}_F$ 

Qubit:

 $\mathcal{H}_q = -\frac{1}{2}B\sigma_z$  - ½-pseudospin in a static "magnetic field"

Fluctuators: 
$$\mathcal{H}_{F} = \mathcal{H}_{F}^{(0)} + \mathcal{H}_{F-env} + \mathcal{H}_{env}$$

Two-level tunneling systems:

$$\mathcal{H}_F^{(0)} = \frac{1}{2} \sum_i E_i \tau_z^i$$

where the Pauli matrices  $\tau^{(i)}$  correspond to *i*-th fluctuator. The spacing between the two levels,  $E_i$  if formed by the diagonal splitting,  $\Delta_i$ , and the tunneling overlap integral,  $\Lambda_i$ 

$$E_i = \sqrt{\Delta_i^2 + \Lambda_i^2} \equiv \Lambda_i / \sin \theta_i$$
.

### Fluctuators (continued):

(boson bath, only flip-flop processes are taken into account)

$$\mathcal{H}_{\text{env}} = \sum_{\mu} \omega_{\mu} \left( \hat{b}_{\mu}^{\dagger} \hat{b}_{\mu} + 1/2 \right) ,$$
  
$$\mathcal{H}_{F-\text{env}} = \sum_{i} \tau_{x}^{(i)} \sum_{\mu} C_{i,\mu} \left( \hat{b}_{\mu} + \hat{b}_{\mu}^{\dagger} \right)$$

Interaction: (only dephasing is taken into account)

$$\mathcal{H}_{qF} = \sum_{i} v_i \sigma_z \tau_z, \quad v_i = g(r_i) A(\mathbf{n}_i) \cos \theta_i.$$

### Crucial simplification:

Low-frequency fluctuations are treated classically, as a set of random telegraph processes produced by different fluctuators, which switch between two states due to interaction with the thermal bath. The random field acting upon qubit can be modeled by a set of random telegraph processes produced by different fluctuators:  $\mathcal{X}(t) = \sum v_i \xi_i(t)$ 



Random telegraph process:

Switching between +1/2 and -1/2 at random times obeying Poissonian statistics with some rate,  $\gamma$ 

 $\langle \xi(t)\xi(0)\rangle = \frac{1}{4}e^{-2\gamma|t|} \rightarrow \langle \xi(t)\xi(0)\rangle_{\omega} = \frac{1}{4}\frac{2\gamma}{\omega^2 + 4\gamma^2}$ 

Random field can be considered as a classical one modulating the energy spacing between qubit's levels

#### Q: Why this model describes 1/f noise?

A: I f we have many fluctuators, then the noise spectrum is

$$\begin{aligned} \langle \mathcal{X}(t)\mathcal{X}(0) \rangle_{\omega} &= \frac{1}{4} \sum_{i} \frac{v_{i}^{2}}{4\cosh^{2}(E_{i}/2T)} \frac{2\gamma_{i}}{\omega^{2} + 4\gamma_{i}^{2}} \\ &\propto T \int d\gamma \, \mathcal{P}(\gamma) \frac{2\gamma}{\omega^{2} + 4\gamma^{2}} \end{aligned}$$

Key point: since  $\gamma$  is due to tunneling or activation it exponentially depends on the smoothly distributed parameters.

$$\mathcal{P}(\gamma) \propto rac{1}{\gamma} \quad o \quad \langle \mathcal{X}(t) \mathcal{X}(0) 
angle_\omega \propto rac{1}{\omega}$$

We calculate the qubit response using the method of stochastic differential equations

Very brief sketch:

In the rotating frame the density matrix

$$\hat{\rho} = \begin{pmatrix} n & -if e^{i\Omega t} \\ if^* e^{-i\Omega t} & 1-n \end{pmatrix}$$

obeys the set of stochastic differential equations:

$$\frac{\partial n}{\partial t} = -2\gamma_q(n-n_0) - F \operatorname{Re} f,$$

$$\frac{\partial f}{\partial t} = i \left[ E_0 + \mathcal{X}(t) - \Omega \right] f - \gamma_q f + \frac{F}{2}(2n-1).$$

$$F - \operatorname{Rabi} \text{ frequency}$$

$$\mathcal{X}(t) \text{ random}$$
deviation of
eigenfrequency

The signal can be expressed through the phase memory functional:

$$\Psi[\beta(t'),t] = \left\langle \exp\left(i\int_0^t \beta(t')\mathcal{X}(t')\right), dt'\right) \right\rangle$$

 $\beta(t)$  depends on the manipulation procedure.

For two-pulse echo:

Methods of the theory of stochastic differential equations provide exact solution to this problem for qubit and a single fluctuator.



# The phase-memory functional obeys the differential equation

$$\frac{d^2\psi}{dt^2} + \left[2\gamma - \frac{d\ln\beta(t)}{dt} - iv\beta(t)\right]\frac{d\psi_{\pm}}{dt} - iv\gamma\psi = 0$$

with initial conditions  $\psi_{\pm}(0) = 1$ ,  $\frac{d\psi_{\pm}}{dt}\Big|_{t=0} = \pm i\beta(0)\frac{v}{2}$ .

The solution depends on the manipulation procedure through the function  $\beta(t)$ , as well on the coupling constant, v, and switching rate,  $\gamma$ .

### The dimensionless parameter is the ratio $~v/\gamma$

At  $v \gg \gamma$  - quantum beatings between two values of inter-level spacing, the decoherence rate is  $\propto \gamma$ .



At  $v\ll\gamma$  - self-averaging (motional narrowing of spectral lines), the decoherence rate  $v^2/\gamma$  - motional narrowing (Klauder&Anderson, 1954)

Fluctuators with  $v\sim\gamma$  are most active!

# Our calculations for a single fluctuator



In first experiments time-averaged signal was measured

How many experimental runs do wee need?



Simulations, 100 runs



The result is qualitatively similar to the experiment on charge echo



FIG. 3. Decay of the normalized amplitude of the echo signal (filled circles) and the FID signal (open circles) compared with estimated decoherence factors  $\langle \exp i\varphi \rangle$  due to the electromagnetic environment (dotted line), the readout process (dashed line), and 1/f charge noise with  $\alpha = (1.3 \times 10^{-3}e)^2$  (dashed line). The two solid lines are estimations for the echo experiment in the presence of the same 1/f charge-noise spectrum (bottom) and that with  $\alpha = (3.0 \times 10^{-4}e)^2$  (top).

#### From Nakamura et al., PRL 2002

- Q: What happens if there are many fluctucators producing 1/f noise?
- A: Generally, one has to add contributions of all fluctuators. That can be done using the so-called Holtsmark method (see details in the additional part). <u>Main ideas:</u>
  - 1. Fluctuators are uncorrelated

$$\Psi[\beta(t), t] = \prod_{i} \psi_{i} = e^{\sum_{i} \ln \psi_{i}} \rightarrow e^{N \langle \ln \psi \rangle}$$
2. N > 1  $\longrightarrow N \langle \ln \psi \rangle_{F} \rightarrow -N \langle 1 - \psi \rangle_{F}$ 

$$\longrightarrow -\int dv \, d\gamma (\mathcal{P}(v, \gamma)) [1 - \psi(v, \gamma|t)]$$

The results crucially depend on the distribution of v and  $\gamma$ 

Usually  $\mathcal{P}(\gamma) \propto 1/\gamma$ , but  $\mathcal{P}(v)$  depends on the interaction mechanism and spatial arrangement of fluctuators.

It is expected that the fluctuators with  $v \sim \gamma$  are most important, and this is why the Gaussian assumption in general does not hold.

Unfortunately, flicker noise and decoherence are determined in general by different fluctuators, this is why the decoherence rate cannot be expressed though the flicker noise spectrum.

One can find some indications of this property in the recent preprint bi I thier et al., cond-mat/0508.

#### How one can decrease the decoherence?

Decoherence is mainly due to charge noise, which causes fluctuations in the effective magnetic field  $B_z$ .

Main idea is to keep the working point very close to the degenerate state.

Single Cooper pair qubit:

$$\Delta = E_c C_g \left( V_g - V_g^{\text{opt}} \right) / e$$

can be adjusted by gate voltage

$$\Delta, v \ll E_J \longrightarrow E_{\pm} = \pm \left( E_0 + \frac{\Delta v}{2E_J} + \frac{v^2}{4E_J} \right), \quad E_0 = \frac{1}{2}E_J + \frac{\Delta^2}{4E_J}$$
At  $\Delta = 0$  quadratic coupling

NTT BRL School, 2005

We have developed a theory of charge fluctuations near the optimal point.





### Model for calculation of T<sub>1</sub>

<u>Assumption</u>: Tunneling between the gate and the trap depends on the state of the qubit:  $\hat{t} = t_0 + \tilde{t}\sigma_z$ 

$$\mathcal{H} = \begin{bmatrix} -\frac{\delta E_{c}}{2} \sigma_{z} - \frac{E_{J}}{2} \sigma_{x} \end{bmatrix} \text{Qubit}$$

$$F \text{luctuator + gate}$$

$$+ \sum_{\alpha} \epsilon_{\alpha} c_{\alpha}^{\dagger} c_{\alpha} + \frac{1}{2} \sum_{\alpha \neq \beta} U_{\alpha\beta} c_{\alpha}^{\dagger} c_{\alpha} c_{\beta}^{\dagger} c_{\beta} + t_{0} \sum_{\alpha \neq \beta} (c_{\alpha}^{\dagger} c_{\beta}^{\dagger} + c_{\alpha} c_{\beta})$$

$$+ \left[ v \sum_{\alpha} c_{\alpha}^{\dagger} c_{\alpha} + \tilde{t} \sum_{\alpha \neq \beta} (c_{\alpha}^{\dagger} c_{\beta}^{\dagger} + c_{\alpha} c_{\beta}) \right] \sigma_{z}$$

Coupling between qubit and fluctuator

After diagonalizing the qubit Hamiltonian one obtains both dephasing and direct transitions leading to  $T_2$  and  $T_1$ 

NTT BRL School, 2005

## Conclusions

- Decoherence by the flicker noise cannot in general be allowed for by the conventional spin-boson model.
- The spin-fluctuator model allows studying decoherence for various qubit manipulations.
- The model predicts different time dependences of the decoherence at small and large time, comparing to the transition time of a typical fluctuator.
- Proper qubit manipulation can substantially decrease the decoherence

