

Stochastic Models of Quantum Decoherence

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Simplifications

► **Orthodox quantum mechanics**

Assume von Neumann's *Mathematical Foundations of QM*.

Some interesting questions I am **not** attempting to answer:

- 0) Can decoherence explain the *measurement problem*?
- 1) Is the *stochastic interpretation* of QM valid?
- 2) Who was right, Bohr or Einstein?



► **Finite-dimensional Hilbert spaces**

No systems with infinitely-many energy eigenstates.

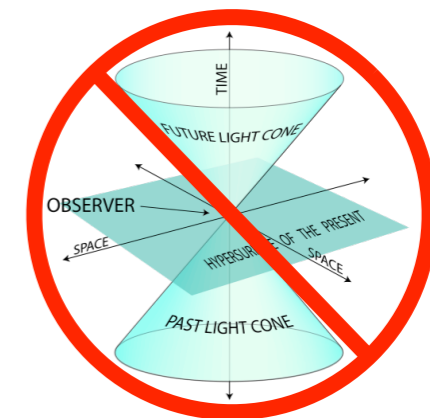
Pure states are column vectors. Operators are matrices.

$$-\frac{\hbar^2}{2m} \nabla^2 \Psi(x, t)$$
$$|a\rangle = \delta(x - a)$$

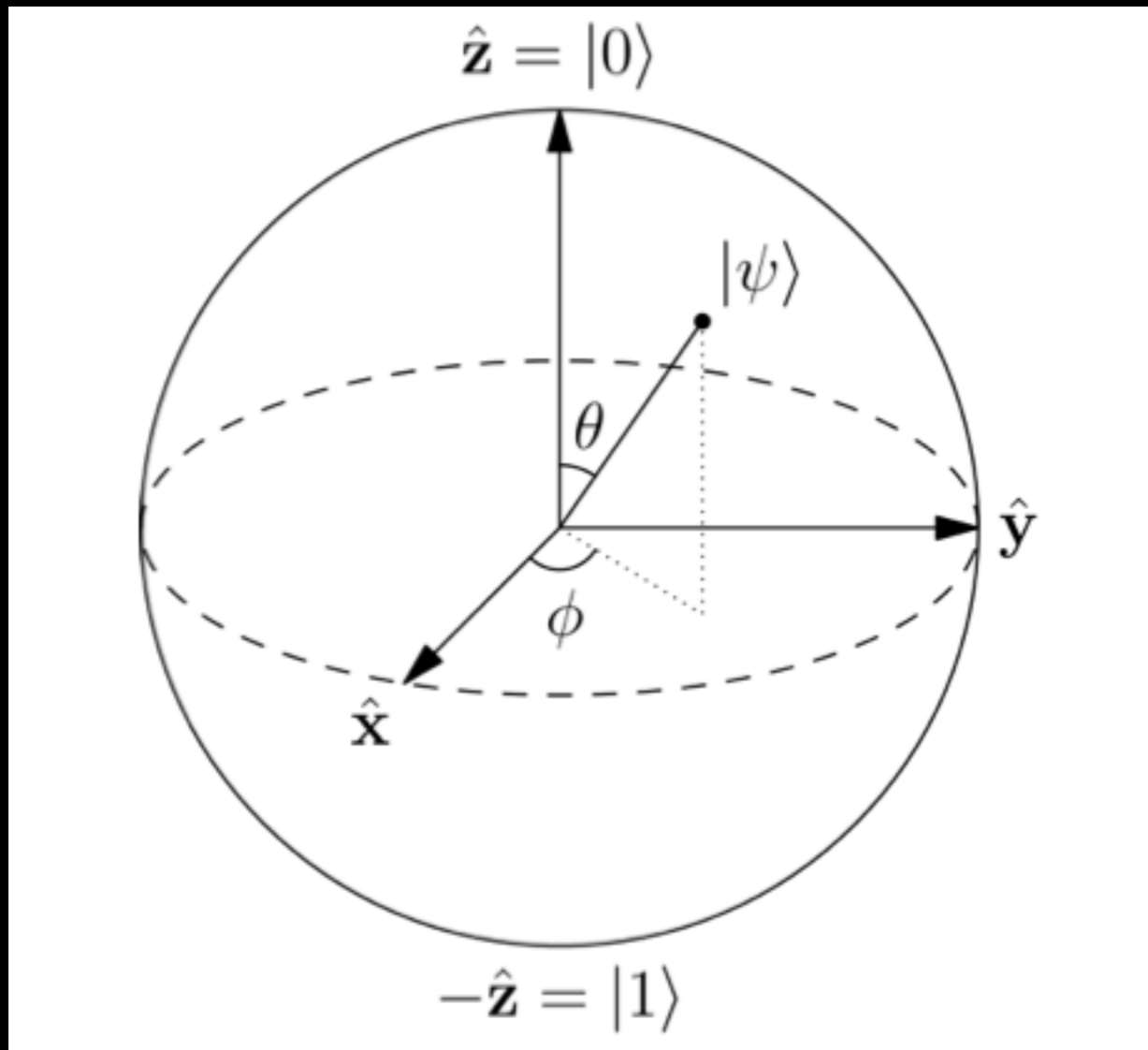
► **No relativity**

The Schrödinger equation is assumed correct.

Quantum fields and Lorentz covariance are ignored.

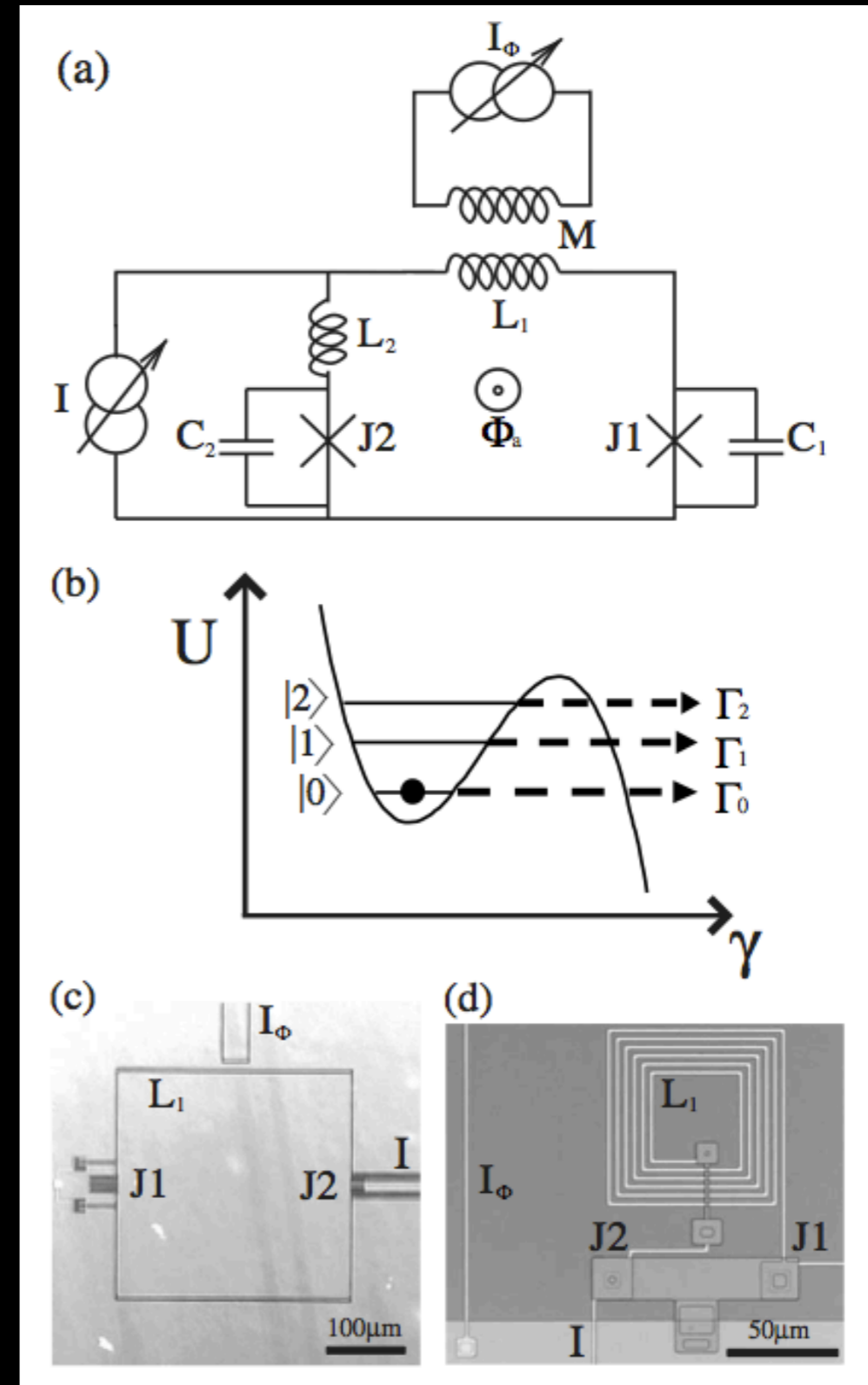


What is a qubit?



Above: Any qubit pure state corresponds to a point on the Bloch sphere.

Right: Example phase qubit design by team at U. of Maryland, College Park. From *Phys. Rev. B*, vol. 77 (2008)



X's in circuit diagram are superconducting Josephson junctions. Don't worry about the details – the point is, real qubits can be complicated things.

Qubit mixed states

- ▶ A **classical bit** is a system with two states named 0 and 1.
- ▶ A **qubit** is a system with two basis states named $|0\rangle$ and $|1\rangle$. Its state can also be a superposition of these basis states:

$$|\Psi\rangle = \alpha|0\rangle + \beta|1\rangle$$

- ▶ **Density matrices** are useful “when we do not even know what state is actually present.” For each possible state, define a **projection operator**:

$$\hat{\rho} \equiv |\Psi\rangle\langle\Psi| = \begin{bmatrix} \alpha^*\alpha & \beta^*\alpha \\ \alpha^*\beta & \beta^*\beta \end{bmatrix}$$

- ▶ If possible state $\hat{\rho}_k$ occurs with probability p_k , then define a **mixed state**:

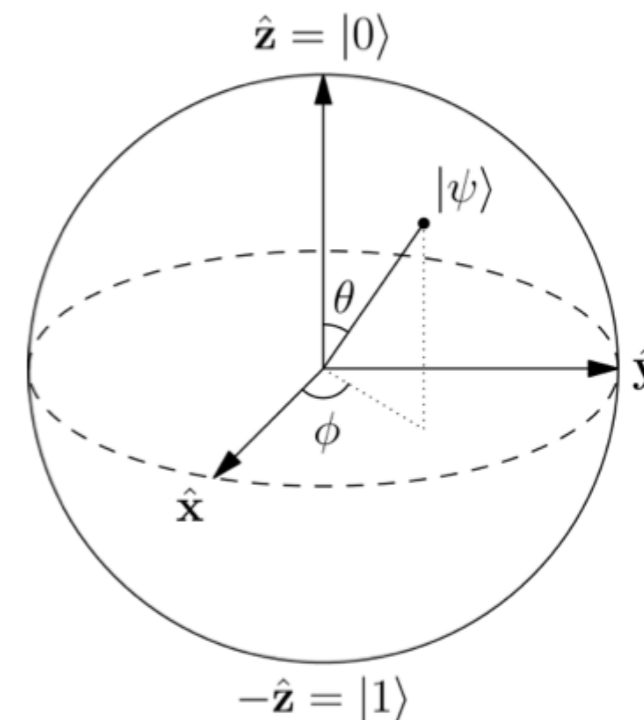
$$\bar{\rho} \equiv E[\hat{\rho}] = p_1\hat{\rho}_1 + p_2\hat{\rho}_2 + \cdots = \sum_k p_k\hat{\rho}_k$$

Qubits as geometric objects

- ▶ **The Bloch sphere** is a common way to visualize qubit states. The ground state is at the North pole. The excited state is at the South pole.
- ▶ **Pure states** are points *on* the sphere.
Mixed states are points *inside* the sphere.
- ▶ Any 2x2 self-adjoint complex matrix is a real linear combination of Pauli matrices and the identity matrix:

$$\frac{1}{2} (w\hat{1} + x\hat{\sigma}_x + y\hat{\sigma}_y + z\hat{\sigma}_z) = \frac{1}{2} \begin{bmatrix} w + z & x - iy \\ x + iy & w - z \end{bmatrix}$$

- ▶ Density matrices have $w = 1$ and $x^2 + y^2 + z^2 \leq 1$.
Define **Pauli coordinates** x, y, z of a (pure or mixed) qubit state this way.
The vector $\mathbf{r} = (x, y, z)$ is the state's Bloch vector in Cartesian coordinates.



Spin-1/2 parameters

- ▶ Time evolution is found by solving the **Liouville-von Neumann equation (LvN)**, which is the density-matrix version of the Schrödinger equation:

$$i\hbar \frac{d}{dt} \bar{\rho} = [\hat{H}, \bar{\rho}]$$

- ▶ **Any qubit can be represented by a fictional spin-1/2 in a magnetic field:**

$$\hbar \frac{d}{dt} \mathbf{r} = -\mathbf{B} \times \mathbf{r}$$

This is equivalent to the LvN equation if B_x, B_y, B_z are the Pauli coordinates of $-\hat{H}$. (The w component does not affect time evolution.)

- ▶ **Measurement probabilities** are found by dot products. For a qubit observable \mathbf{A} (in Pauli coordinates), the probability of an “up” or “down” result is:

$$\frac{1}{2} \left(1 \pm \mathbf{r} \cdot \frac{\mathbf{A}}{|\mathbf{A}|} \right)$$

The w component does not affect these either.

Canonical mixed states

- ▶ The **von Neumann entropy** of $\bar{\rho}$ is the Shannon entropy of its eigenvalues:

$$S(\bar{\rho}) \equiv -\text{Tr}[\bar{\rho} \log(\bar{\rho})] = -\sum \lambda_n \log(\lambda_n)$$

S is zero for pure states. For qubits, it depends on radius only.

- ▶ S is used to calculate thermal equilibrium **canonical mixed states**:

$$\bar{\rho}_\beta = \frac{1}{2 \cosh(\frac{1}{2}\beta\epsilon)} \begin{bmatrix} e^{\frac{1}{2}\beta\epsilon} & 0 \\ 0 & e^{-\frac{1}{2}\beta\epsilon} \end{bmatrix} \quad \beta \equiv \frac{1}{kT}$$

β is inverse temperature, a.k.a. “greed for energy,” and $\epsilon \equiv (E_1 - E_0)$.

- ▶ In Pauli coordinates, **canonical qubit mixed states are on the z-axis**.

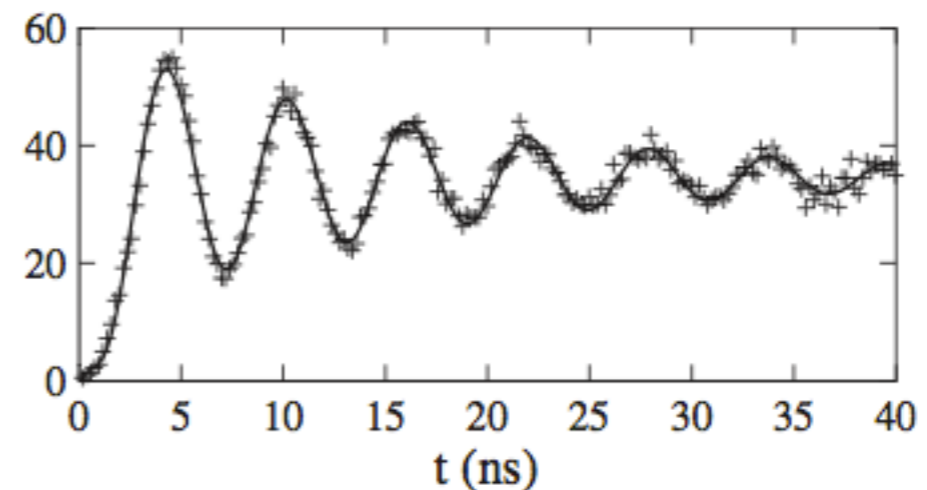
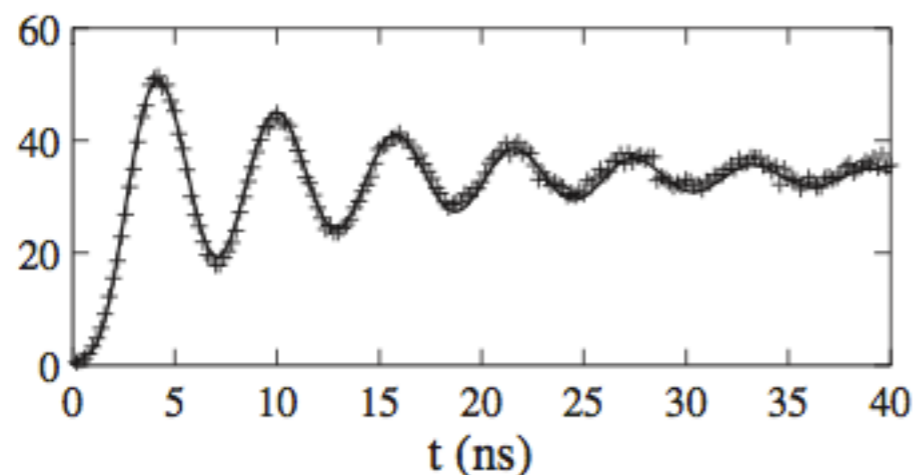
$$\mathbf{r}_\beta = (0, 0, \tanh(\frac{1}{2}\beta\epsilon))$$

In the limit $\beta \rightarrow 0$, the canonical mixed state is $\mathbf{0}$.

Decoherence

► Decoherence

Qubits in real experiments appear to degrade from pure to mixed states.



Both images are Rabi oscillation tests from *Phys. Rev. B*, vol. 77 (2008).

Theory: Undamped sinusoidal oscillations. Experiments: Exponential decay!

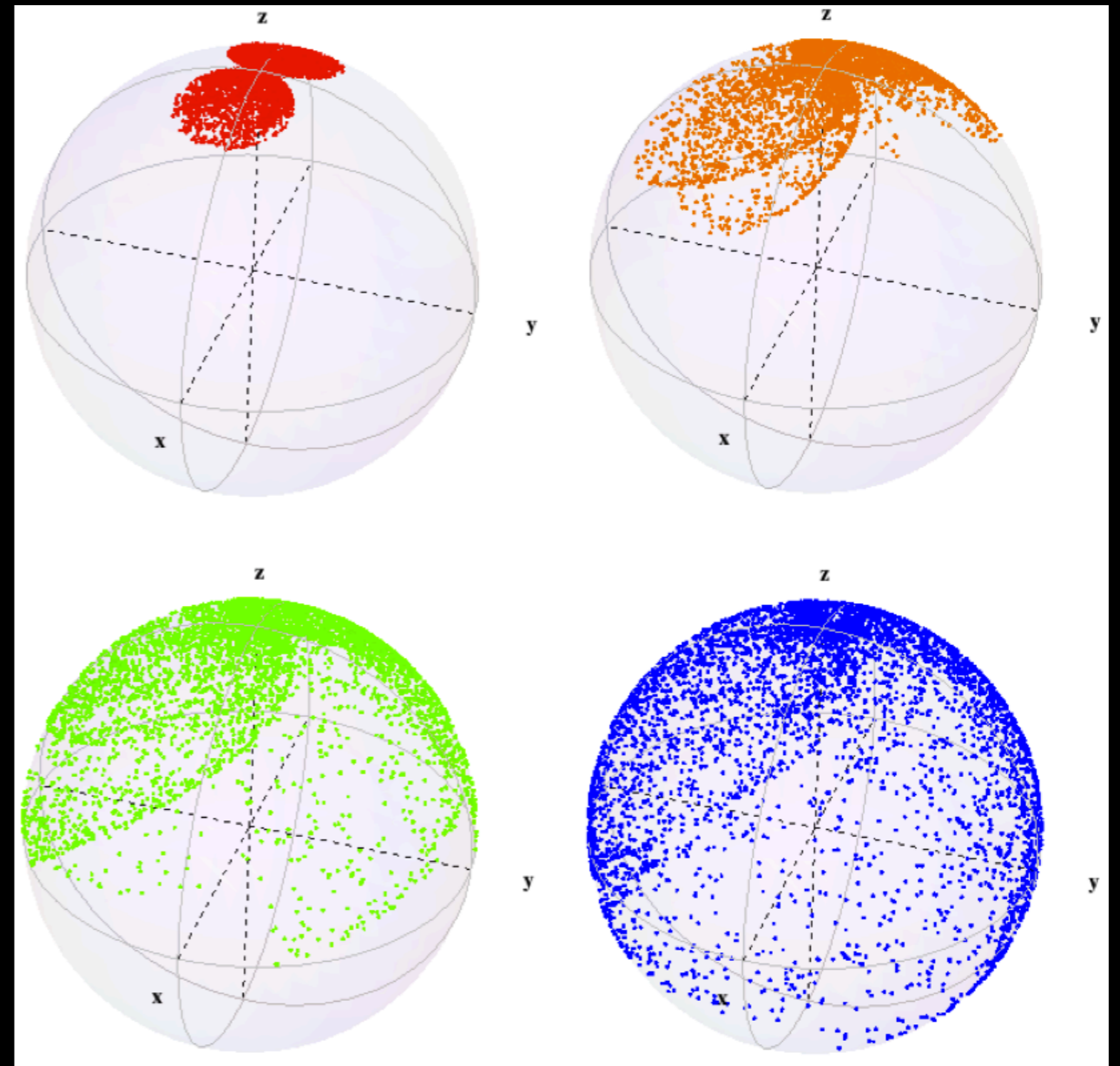
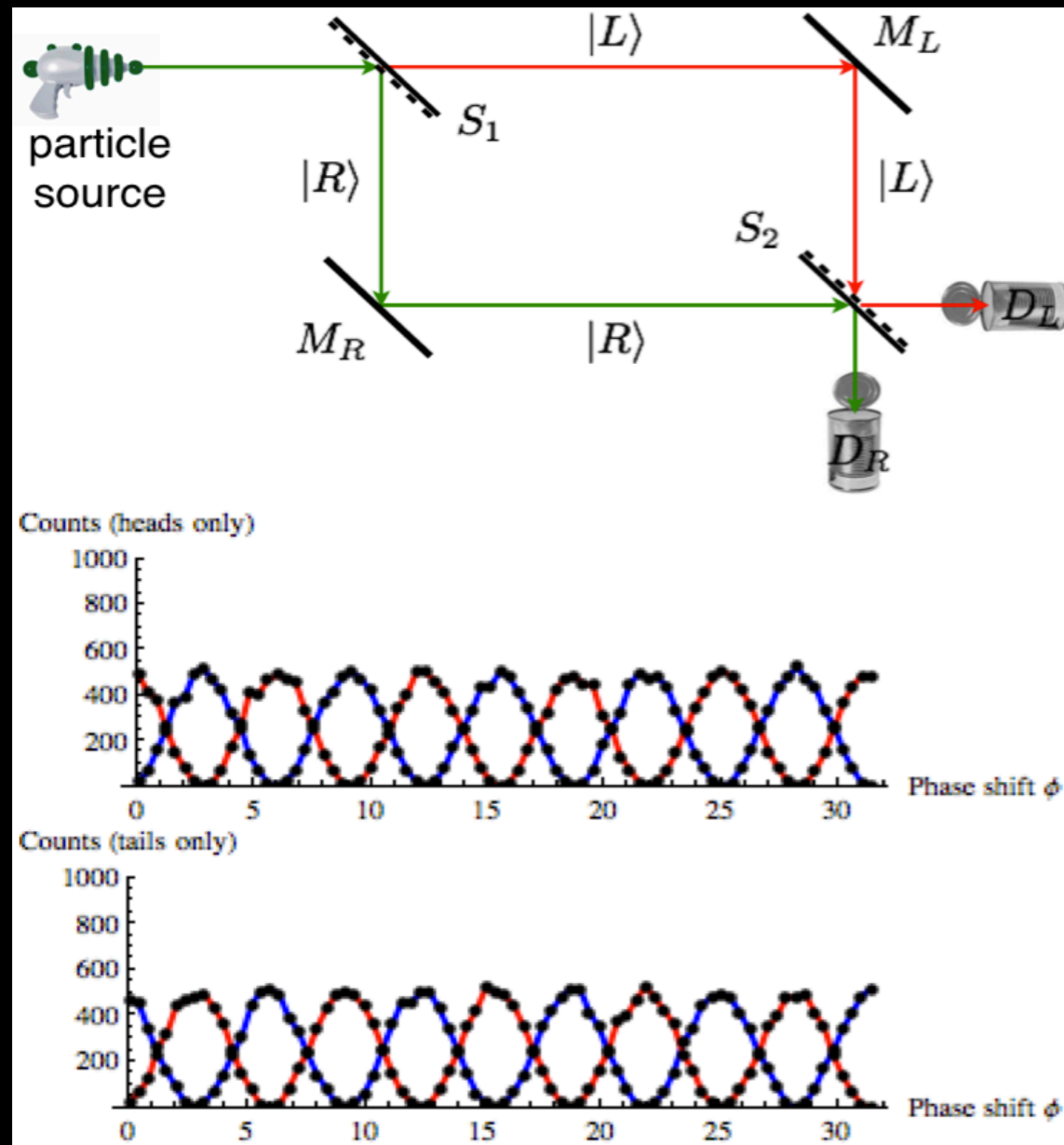
► Quantum Loschmidt paradox: irreversible change from reversible equations?

0) Schrödinger and Liouville-von Neumann equations are time-reversible.

States evolve by unitary transformations which conserve von Neumann entropy.

1) Experiments routinely show irreversible entropy production.

Illusory decoherence



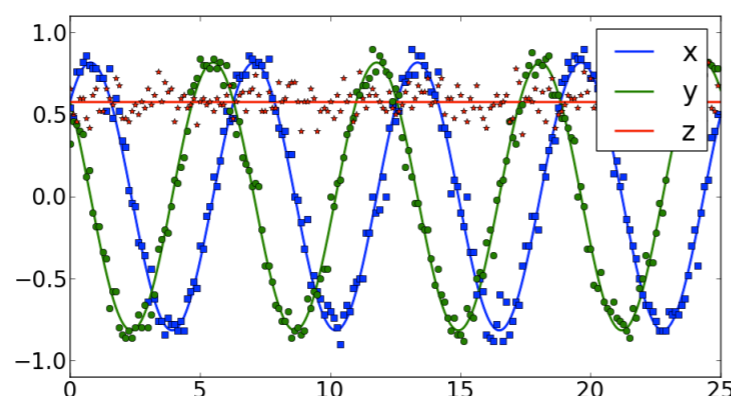
Left: Mach-Zehnder neutron interferometer from *Allyson's Choice* thought experiment and Allyson's decrypted detector count data.

Right: Monte Carlo simulations of *Zech's Qubit* thought experiment color-coded by stray field strength. (Red is weakest, blue is strongest.)

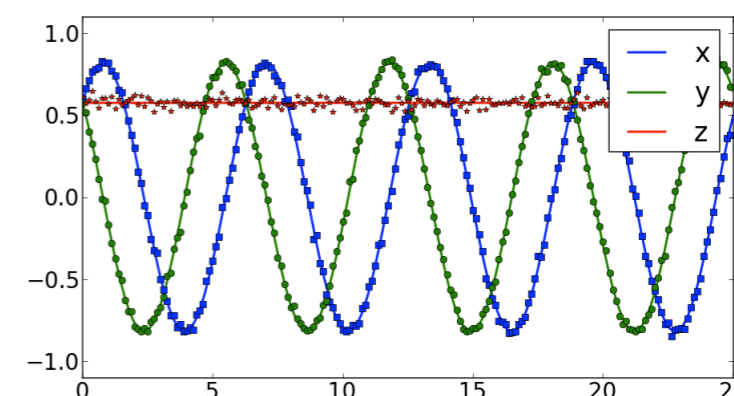
Inferring the state of a qubit

- ▶ The **Law of Large Numbers** can be used to infer a qubit state. A qubit is evolved for some time t , and an observable (e.g. $\hat{\sigma}_z$) is measured. If many independent, identical trials are performed, the average of all results converges to its expected value. In this example, it's $\text{Tr}[\hat{\rho}\hat{\sigma}_z] = z$.
- ▶ **Fluctuations** can appear due to sample-size statistical errors. No laboratory has enough graduate students to perform ∞ experimental trials.

estimated
 x, y, z with
100 trials:



estimated
 x, y, z with
1000 trials:



- ▶ **Dissipation** can appear due to non-identical trials. If we don't know what state is actually present on each trial, we can represent it as a random variable. Measurement probabilities are found by the **Law of Total Probability**:

$$\sum_k p_k \frac{1}{2} \left(1 \pm \mathbf{r}_k \cdot \frac{\mathbf{A}}{|\mathbf{A}|} \right) = \frac{1}{2} \left(1 \pm \bar{\mathbf{r}} \cdot \frac{\mathbf{A}}{|\mathbf{A}|} \right) \quad \bar{\mathbf{r}} \equiv \sum_k p_k \mathbf{r}_k$$

True states, mean states, and estimated states

- ▶ Assume the **true state of a system** is always pure on each trial: $|\mathbf{r}_k(t)| = 1$
- ▶ The **mean state of a model** is the expectation value of the true state:

$$\bar{\mathbf{r}}(t) \equiv E[\mathbf{r}(t)] = \sum p_k \mathbf{r}_k(t)$$

Qubit mean states are points on *or inside* the Bloch sphere: $|\bar{\mathbf{r}}(t)| \leq 1$
Not-identical trials \Rightarrow mean state can gain entropy!

- ▶ Components of the **estimated state of a dataset** are the sample means X, Y, Z of Pauli coordinates x, y, z . Estimated states are points inside a *cube*:

$$X \in [-1, 1] \quad Y \in [-1, 1] \quad Z \in [-1, 1]$$

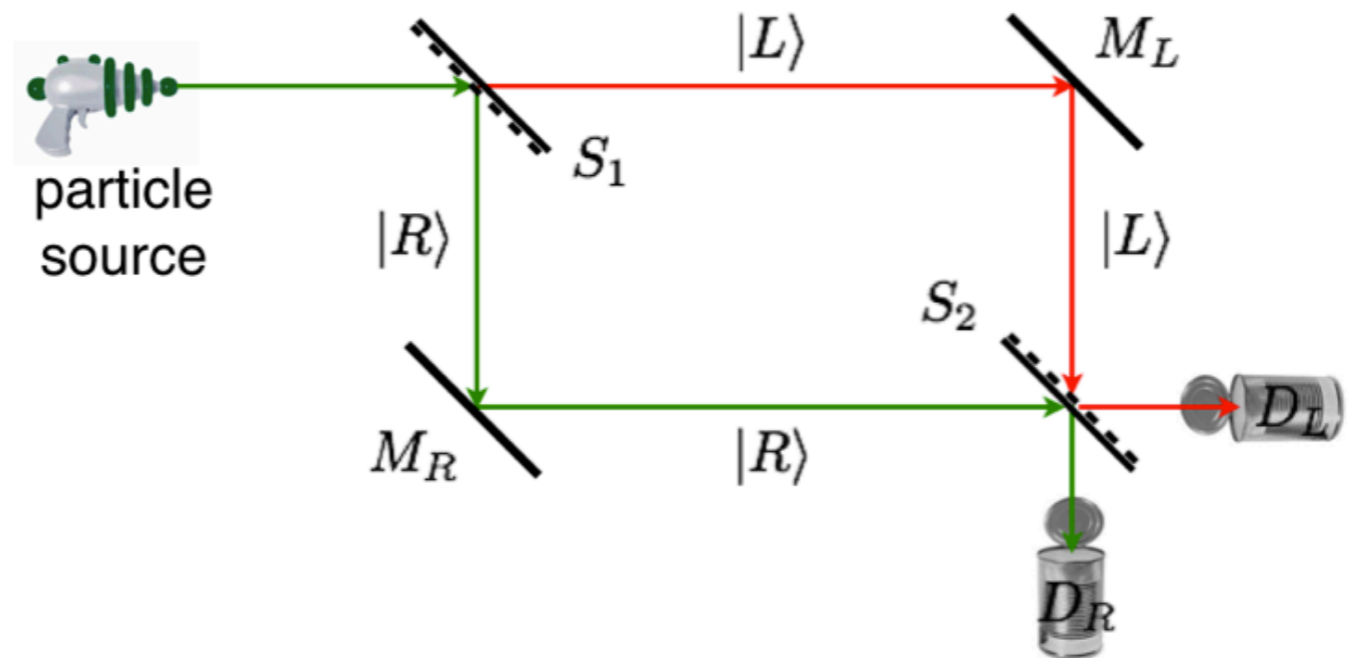
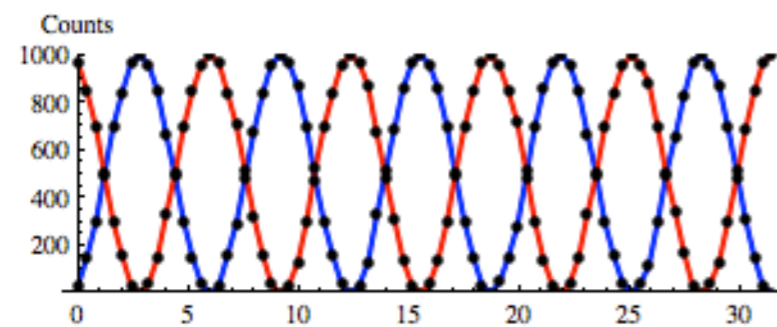
- ▶ An estimated state is a *maximum likelihood estimator*, not a physical state. In the limit of many trials, **estimated states converge to the mean state**. Statistical estimators can gain entropy even if true states are always pure.

Allyson's Choice thought experiment

▶ Bob's intended experiment

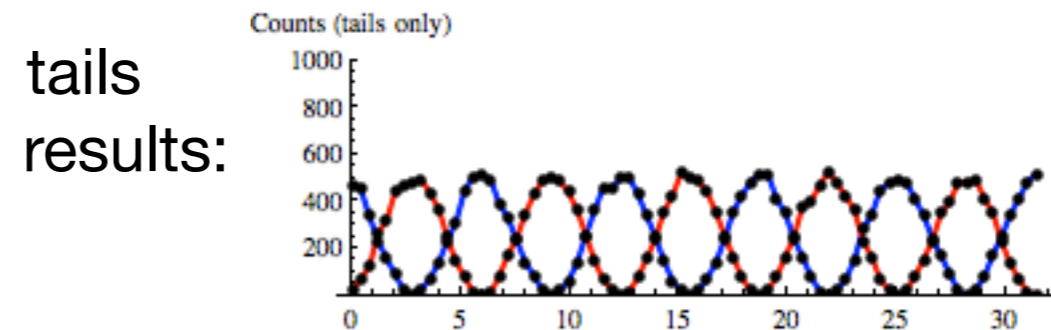
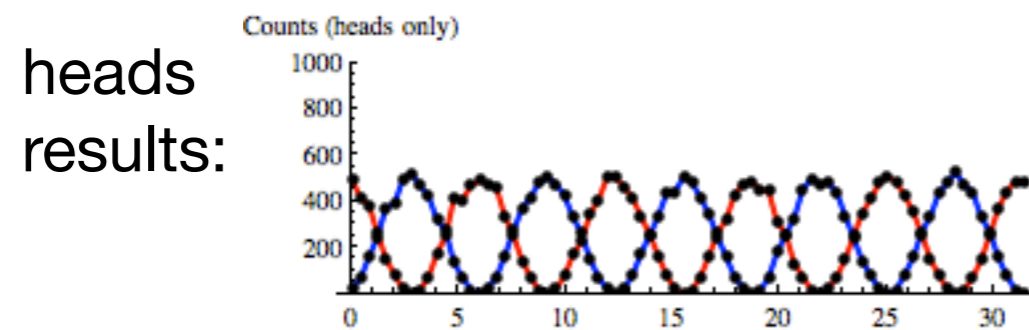
Professor Bob sends a neutron through a Mach-Zehnder interferometer. The neutron's wavefunction acquires a phase shift along either path.

Plot of detector counts vs. phase difference φ :



▶ Allyson's shenanigans

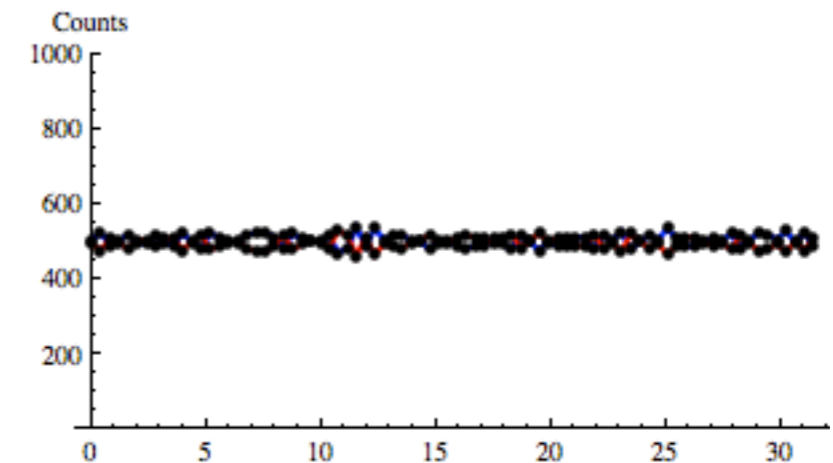
On each trial of the experiment, Allyson flips a fair coin. If heads, she does what Bob says. If tails, she reverses the orientation of \hat{S}_2 .



Information was encrypted, not destroyed

- ▶ **Bob sees decoherence**

Bob's plot shows no evidence of de Broglie interference. His students conclude that QM is wrong and classical mechanics rules.



- ▶ **Allyson can decrypt the data**

Allyson can partition Bob's data into "heads only" and "tails only" subsets. Each of those datasets shows: QM rules, classical mechanics is wrong.

- ▶ **...unless she forgets the password!**

To partition the data, Allyson needs to know the results of her coin tosses. She has encrypted Bob's data with a provably-secure *one-time pad*.

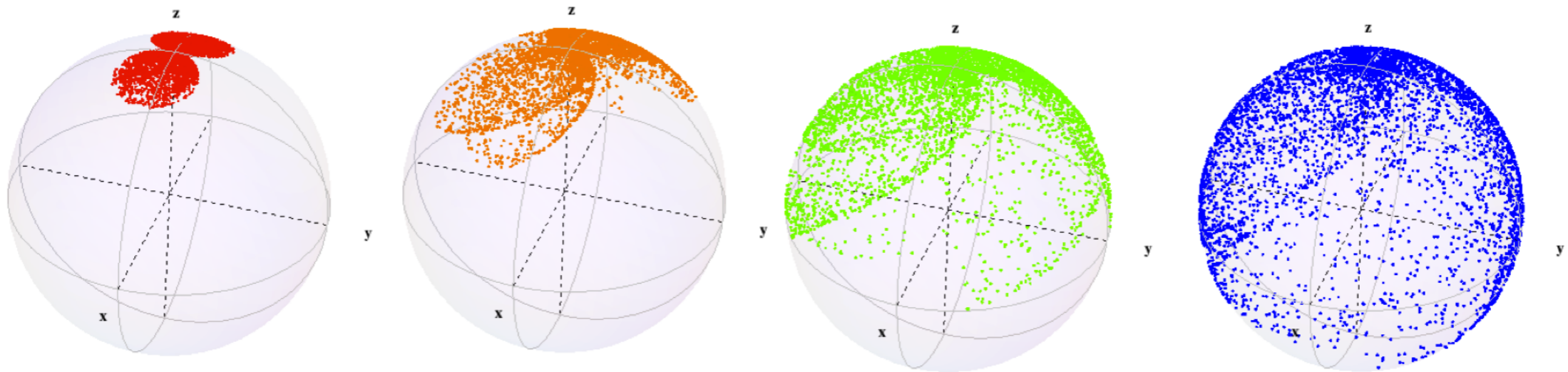
- ▶ **Decoherence by 1000 small cuts**

Suppose Allyson and Bob do the experiment again the way Bob intended, but now φ is random and normally-distributed on each trial. The mean state is:

$$\bar{\mathbf{r}} = E[\mathbf{r}] = \left(0, \sin(\mu)e^{-\frac{1}{2}\sigma^2}, -\cos(\mu)e^{-\frac{1}{2}\sigma^2} \right)$$

Zech's qubit

- ▶ **Zech's qubit** is a spin- $\frac{1}{2}$ in a uniform, constant \mathbf{B} field in the z direction. At time $t=0$, a stray field in the x direction "leaks" through the qubit's shielding. The amplitude and duration of the stray field are random and uniformly-distributed on some intervals. Monte Carlo simulations of 5000 possible states are below:



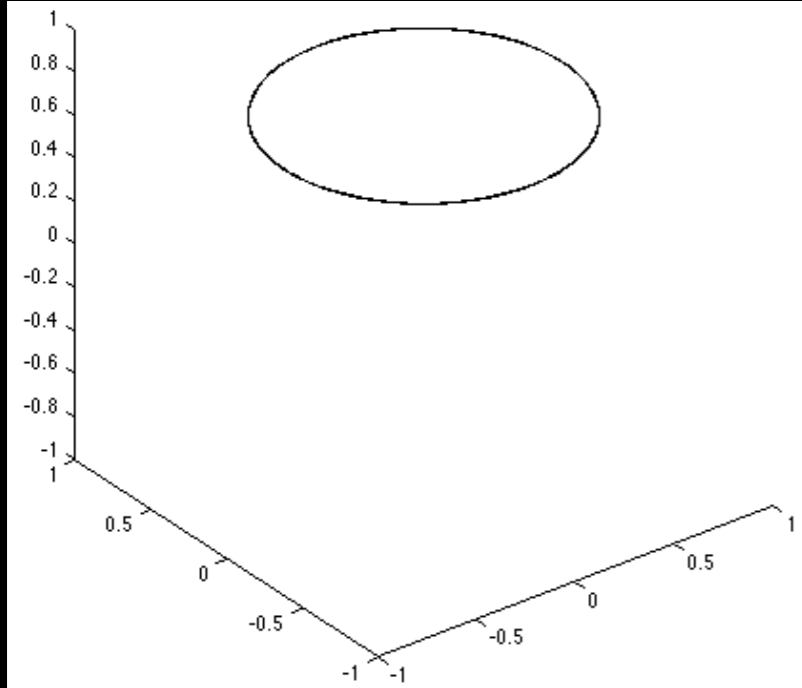
Colors indicate maximum possible stray-field strength. (Blue is strongest.)

- ▶ If $B_x \in [-\mathcal{B}, \mathcal{B}]$, then in the long-duration limit, the mean state is:

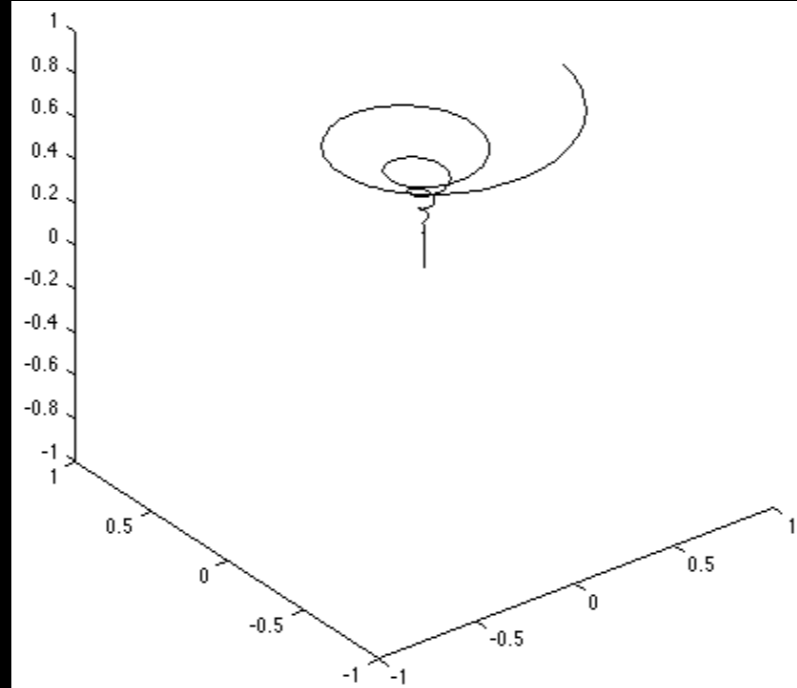
$$\bar{\mathbf{r}} = \left(0, 0, \frac{1}{\mathcal{B}} \arctan(\mathcal{B}) \right)$$

- ▶ If Zech has recorded the amplitude and duration of the stray field, then he can reverse its effect. These numbers are the password for unscrambling his qubit.

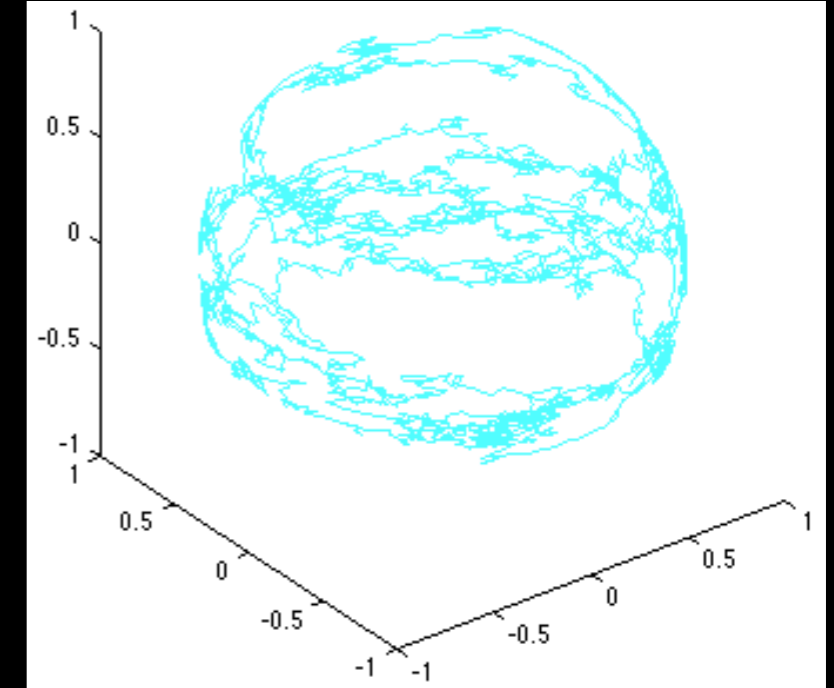
Drunk qubits



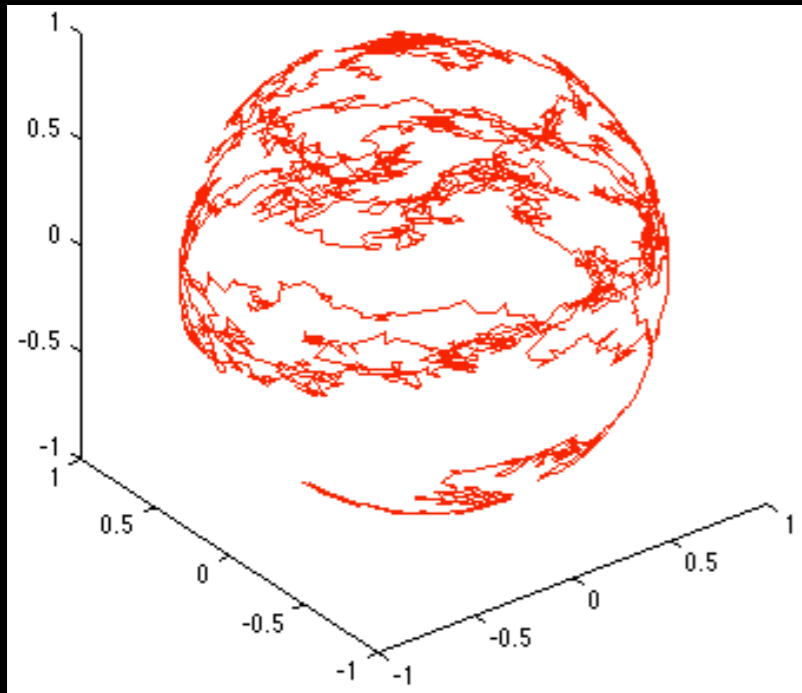
What theory says they do



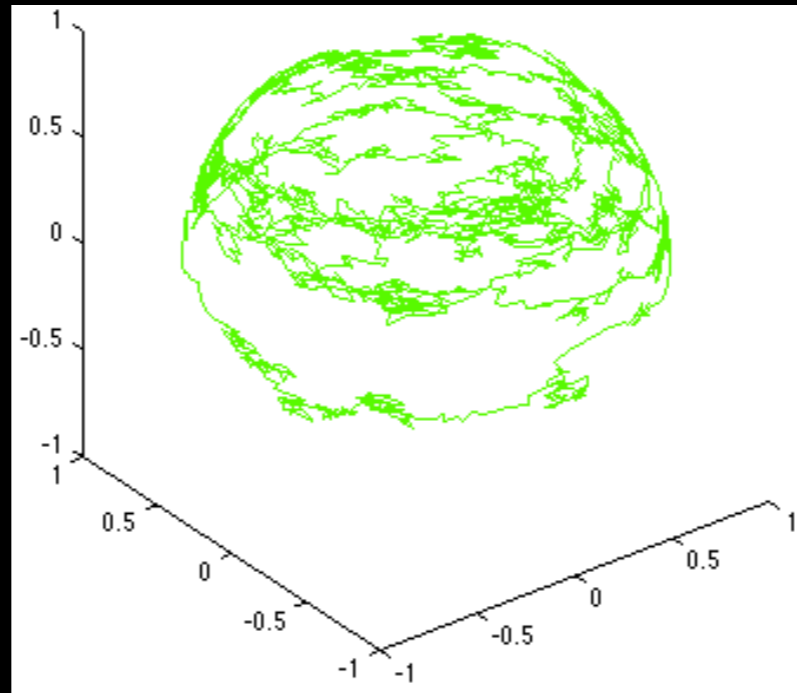
What experiments say they do



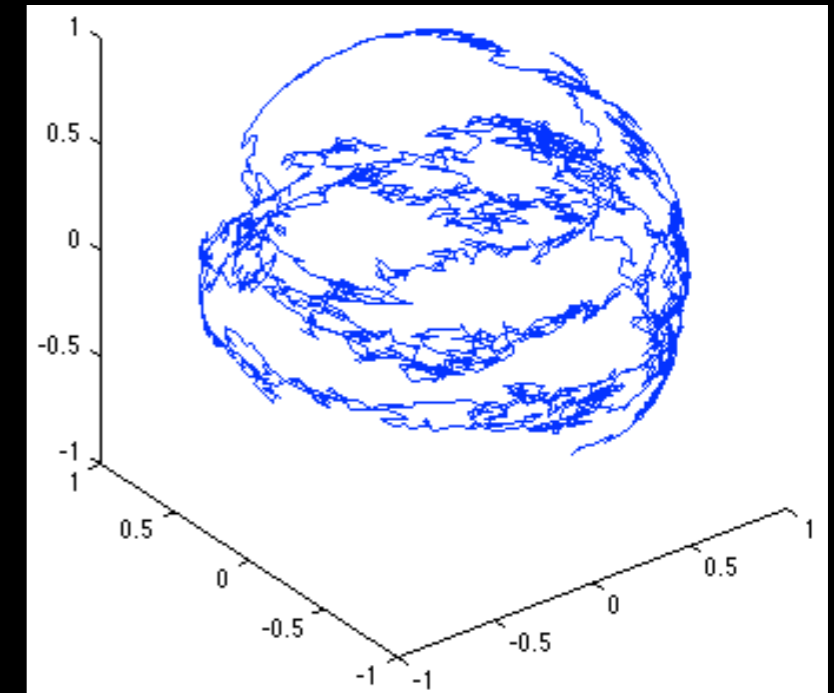
What they really do



or maybe this...



or sometimes this...



or something like this...

If I have to describe the thesis with one slide, this is it.

Stochastic differential equations (SDEs)

- ▶ For more realistic models, use **stochastic processes** which change in time.

$$\frac{d\mathbf{r}_t}{dt} = -\mathbf{B}_t \times \mathbf{r}_t \quad \mathbf{B}_t = \boldsymbol{\mu}(t, \mathbf{r}_t) + \hat{\Sigma}(t, \mathbf{r}_t) \frac{d\mathbf{W}_t}{dt}$$

The **mean field** $\boldsymbol{\mu}$ is a real 3x1 column vector, the **volatility matrix** Σ is a real 3x3 matrix, and \mathbf{W}_t is a real 3x1 column of independent *Wiener processes*.

- ▶ $\frac{dW_t}{dt}$ is a useful heuristic for Gaussian white noise, but it is ambiguous because the Wiener process is not differentiable. **Stochastic calculus** is required.
- ▶ If we use **Itô calculus**, then the Chain Rule must be replaced by **Itô's Lemma**:

$$df(t, W_t) = \left[\dot{f}(t, W_t) + \frac{1}{2} f''(t, W_t) \right] dt + f'(t, W_t) dW_t$$

- ▶ If we use **Stratonovich-Fisk calculus (SF)**, then the ordinary Chain Rule works, but expectation values are harder to calculate. For equations of the form above, we *must* use SF calculus to keep states on the Bloch sphere.

The drunken master equation

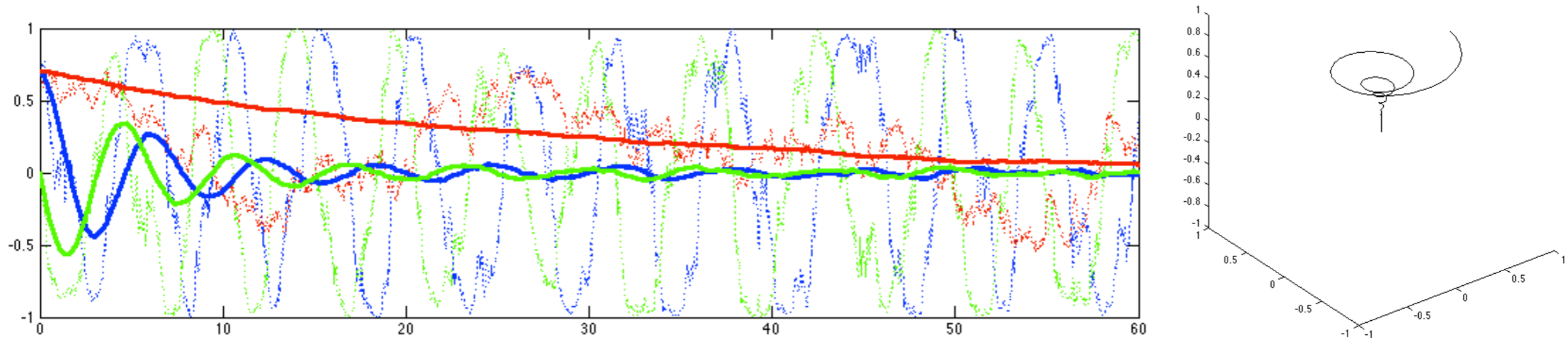
- ▶ For every SF SDE, there is an Itô SDE with the same solution and vice versa. Converting from SF to Itô form provides a shortcut for calculating mean states.
- ▶ For **linear drunk models**, $\boldsymbol{\mu}$ and Σ do not depend on \mathbf{r} . The mean state obeys an ordinary differential equation which I call the **drunken master equation**:

$$\frac{d}{dt}\bar{\mathbf{r}} = -\boldsymbol{\mu} \times \bar{\mathbf{r}} + \frac{1}{2} \left(\hat{\Sigma}^T \hat{\Sigma} - \text{Tr}[\hat{\Sigma}^T \hat{\Sigma}] \hat{\mathbf{1}} \right) \bar{\mathbf{r}}$$

- ▶ The **Bloch equation** from NMR is commonly used to model decoherent qubits. It predicts exponential decay of $\mathbf{r}(t)$ to an equilibrium state on the z axis.
- ▶ If the equilibrium state is $\mathbf{0}$, then the Bloch equation is a special case of the drunken master equation. To derive it, set the volatility matrix Σ to:

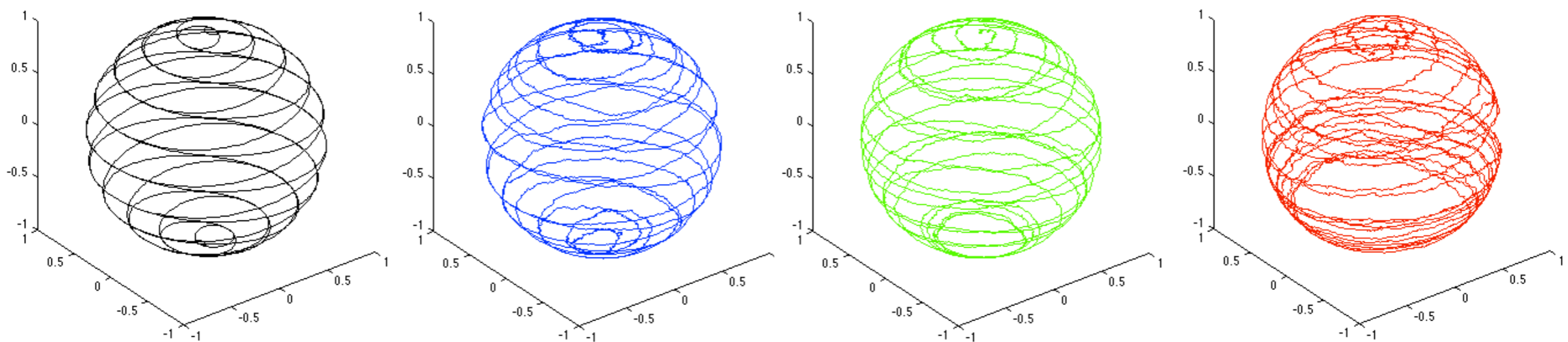
$$\hat{\Sigma} = \begin{bmatrix} \nu_1 & 0 & 0 \\ 0 & \nu_1 & 0 \\ 0 & 0 & \nu_z \end{bmatrix} \quad \nu_1 = \sqrt{\frac{1}{T_1}} \quad \nu_z = \sqrt{\frac{2T_1 - T_2}{T_1 T_2}}$$

Simulations using the linear Bloch model



Left: Pauli coordinates $x(t)$, $y(t)$, $z(t)$ for mean state (solid lines) and one simulated true state (dotted lines). Right: Mean state trajectory. Both use $\mu = (0, 0, 1)$.

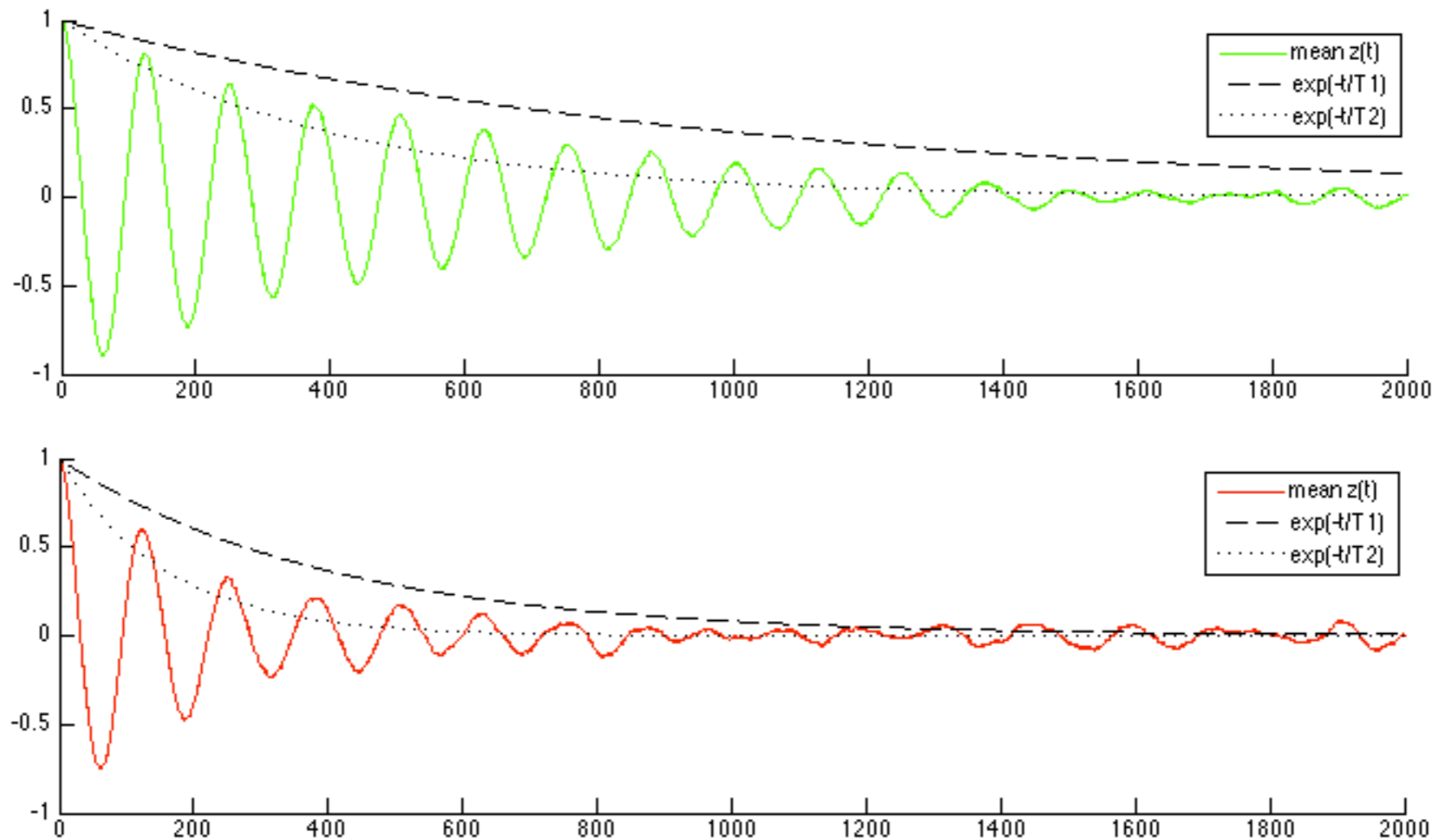
Below: Simulated true states for one full Rabi cycle starting at North pole. Black is noise-free. Colors indicate low, medium, and high volatility.



Black is sober, blue had a glass of wine, green had a few, and red needs help getting home.

Simulated Rabi cycles

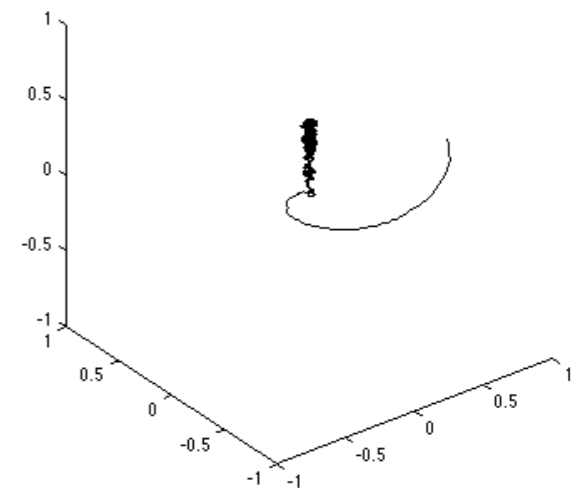
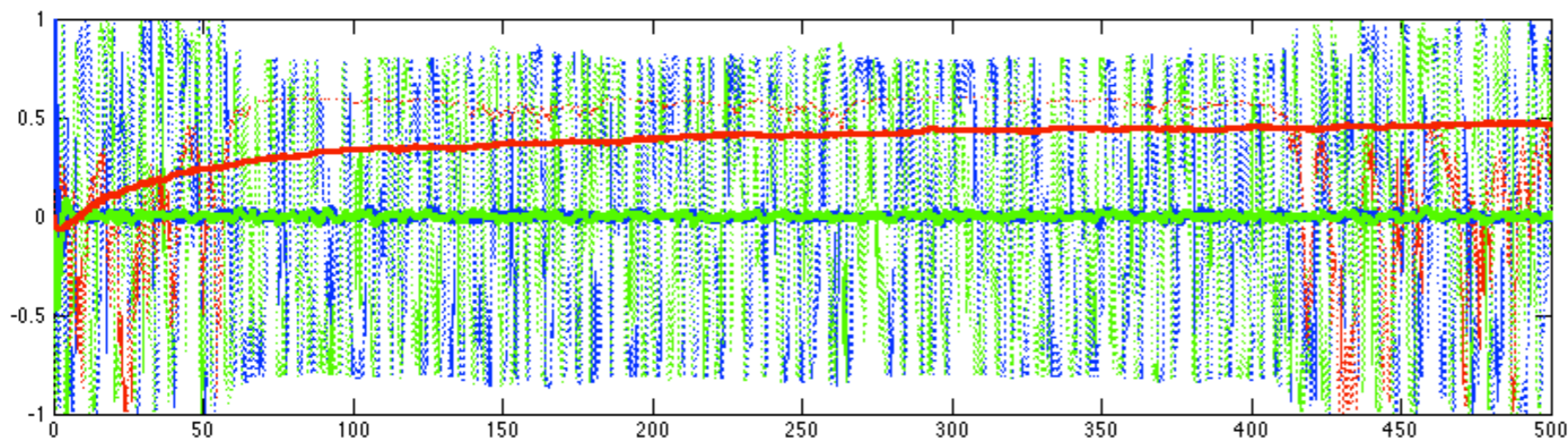
- ▶ **Rabi cycles** result from applying a weak oscillating **B** component in the **x** direction at the qubit's natural frequency $\omega_0 = (E_1 - E_0)/\hbar$. Ideally, the qubit's **z** coordinate oscillates indefinitely.



Above: Monte Carlo simulated Rabi cycles. Colors are **medium** and **high** volatility.

Nonlinear drunk models

- ▶ For nonsingular Σ , linear models have no steady-state solution except $\bar{\mathbf{r}} = \mathbf{0}$.
- ▶ If μ and/or Σ depend on the qubit's state r , then the SDE is nonlinear. The drunken master equation is not valid for nonlinear models.
- ▶ Monte Carlo simulations are still possible. This example **surplus energy model** has a diagonal volatility matrix Σ which is singular when $z = 0.6$. The mean state of this model appears to approach a canonical mixed state on the z axis.



Left: Pauli coordinates $x(t)$, $y(t)$, $z(t)$ for mean state (solid lines) and one simulated true state (dotted lines). Right: Mean state trajectory. Both use $\mu = (0, 0, 1)$.

Note that the sample state (dotted lines in the time series) gets “stuck” near $z=0.6$, but it eventually breaks free.

A loophole in Loschmidt's paradox



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Loschmidt asked how Boltzmann's H-theorem derived irreversible change from reversible classical mechanics. Short answer: Boltzmann averaged over some random terms.

Anthropomorphic entropy and the shuffle hypothesis

- ▶ **Drunk models do not define the “entropy of a qubit.”** Entropy is assigned only to mean states, estimated states, and random variables.
- ▶ Jaynes advocated a more general version of the same idea:

“It is possible to maintain the view that the system is at all times in some definite but unknown pure state... it is not the physical process that is irreversible, but rather our ability to follow it.” *Phys. Rev.*, vol. 108, no. 2 (1957)
- ▶ Jaynes said he got this idea from Wigner’s phrase “entropy is an anthropomorphic concept.” Eddington’s **shuffle hypothesis** is similar:

“Whenever anything happens which cannot be undone, it is always reducible to the introduction of a random element analogous to that introduced by shuffling.” *The Nature of the Physical World* (1929)
- ▶ Shuffles are reversible permutations, but a good shuffle irreversibly degrades players’ ability to predict the order of the cards. Shuffles, encryption, and drunk models are **reversible in principle but seem irreversible in practice.**

Drunk models decoherence is “fake”

- ▶ The word “decoherence” has acquired various different definitions. Joos, et al. define it as **damping of off-diagonal density matrix terms** in some basis. They suggest partitioning decoherence into 3 categories (my paraphrasing):
 1. **True decoherence:** The qubit we’re describing has become entangled with its environment. The (qubit U environment) state is not a direct product of a qubit state and an environment state.
 2. **False decoherence:** The state of our qubit happens to be $|0\rangle$ or $|1\rangle$ right now. In this case, off-diagonal terms of ρ disappear even for pure states.
 3. **Fake decoherence:** We averaged over some ensemble of states.
- ▶ According to these definitions, **drunk models describe fake decoherence.** Mean states are averages over possible true states. Estimated states are averages of measurement counts. To accurately describe “true” decoherence, we need a mathematical representation of our qubit’s environment.

Kossakowski-Lindblad master (KLM) equations

- ▶ **KLM equations** describe linear non-unitary time evolution of systems. The (qubit U environment) system evolves unitarily. A *partial trace* is taken over uncontrolled degrees of freedom. KLM equations are of the form:

$$\hbar \frac{d}{dt} \bar{\rho} = -i [\hat{H}, \bar{\rho}] + \frac{1}{2} \sum_{n,m=1}^{N^2-1} c_{nm} \left([\hat{L}_n, \bar{\rho} \hat{L}_m^\dagger] + [\hat{L}_n \bar{\rho}, \hat{L}_m^\dagger] \right)$$

where $\{\hat{L}_n\}$ are traceless operators which are Hilbert-Schmidt orthogonal, and $\{c_{nm}\}$ are coefficients of a positive (possibly complex) matrix.

- ▶ **Qubit drunken master equations are KLM equations.** Written in terms of Pauli coordinates, a drunken master equation is a KLM equation with:

$$\mathbf{B} = \mu \quad \hat{C} = \frac{1}{2} \hat{\Sigma}^T \hat{\Sigma}$$

- ▶ **Not all KLM equations are drunken master equations.** All KLM equations are linear, and some have a nonzero steady-state solution. Linear drunk models cannot have a nonzero steady-state solution.

Conclusions and future work

- ! Drunk models provide a **quantitative formalism for “fake” decoherence** caused by non-identical trials during qubit experiments.
- ! Drunk models use **unitary evolution to predict the *appearance* of decoherence**, which avoids the quantum Loschmidt paradox.
- ! The only equilibrium mean state for linear drunk models is **0**. **Except for this disagreement, the Bloch equation can be derived from a drunk model.**
- ? Simulations suggest nonlinear drunk models can evolve to a canonical mixed state, but they need not obey a linear master equation. Is this useful?
- ? Every qubit drunken master equation is a Kossakowski-Lindblad master equation. Do linear drunk models and KLM disagree for N -level systems?
- ? How do we model noise that is not Gaussian, not white, and/or not Markovian? (This is a very difficult mathematical question, and not just for qubits!)

The last word

“You should call it *entropy*, for two reasons. In the first place your uncertainty function has been used in statistical mechanics under that name, so it already has a name. In the second place, and more important, **nobody knows what entropy really is**, so in a debate you will always have the advantage.”

- John von Neumann, to Claude Shannon