Stochastic processes in Hilbert space: an introduction to the stochastic Schrödinger equation

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Outline

Two intertwined motivations

The macroscopic objectification problem

The problem:

"*the very possibility of performing measurements on a microsystem combined with the assumed general validity of the linear nature of quantum evolution leads to a fundamental contradiction*" Bassi and Ghirardi, *Physics Letters A*, (2000)

Proposed way out (list not complete):

- von Neumann-Pauli-Lüders postulate (standard, F.A.P.P.)
- Decoherence
- Alternative theory (e.g. D. Bohm)
- Modifications of Q.M. (G.R.W, Gisin, Pearle)

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Effective description Open Quantum System

The problem: a physical system is never really isolated but always interacts with the surrounding environment.

- Standard Quantum Mechanics describes closed systems.
- Contemporary experiments require modeling interaction with the environment.
- Detailed description of the environment computationally very hard and physically not relevant.
- Need of an effective description of the system.

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The F.A.P.P. postulates of Quantum Mechanics

"Kinematic" postulates

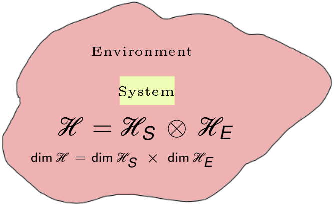
Remark: A Hilbert space $\mathscr{H} \approx \mathbb{C}^d$ is enough for "most" of Q.M. (e.g. $d = 2$)

States and Operators

- System $\Leftrightarrow$ unit ray ψ , in a Hilbert space $\mathscr{H} \subseteq \mathbb{C}^d$: $\psi^\dagger \psi = \sum_{i=1}^{d} \psi_i^* \psi_i = 1$
- Measurable quantity $\Leftrightarrow$ linear self-adjoint operator $\mathbb{A}$ on $\mathscr{H}$: if the spectrum of $\mathbb{A}$ is non-degenerate
  - possible measurement outcomes are the eigenvalues $\{a_i\}_{i=1}^{d}$ of $\mathbb{A}$
  - $\mathrm{Prob}(a_i) = |v_{a_i}^\dagger \psi|^2 = \mathrm{Tr}(\psi \psi^\dagger \, v_{a_i} \, v_{a_i}^\dagger)$ for $\mathbb{A} v_{a_i} = a_i \, v_{a_i}$

Composite system postulate

- The state space is the tensor product of the state spaces of the component physical systems



Dynamic postulate I

Unitary evolution of pure states (Schrödinger eq.)

$$\left.\begin{array}{l} \imath\,\partial_t\psi(t) = \mathbb{H}\,\psi(t) \\ \psi(0) = \psi_o \end{array}\right\} \quad \Rightarrow \quad \psi(t) = \mathbb{U}_t\,\psi_o$$

Unitary evolution of mixtures (Liouville-von Neumann eq.)

$$\left.\begin{array}{l} \imath\,\partial_t\rho(t) = [\mathbb{H}\,,\rho(t)] \\ \rho(0) = \sum_i c_i\psi_{o,i}\psi_{o,i}^{\dagger} \end{array}\right\} \quad \Rightarrow \quad \rho(t) = \mathbb{U}_t\,\rho(0)\,\mathbb{U}_t^{\dagger}$$

$c_i =$ epistemic probabilities.

Remark: $\hbar = 1$ everywhere.

Entanglement and the intertwined motivations

The problem with multipartite system description

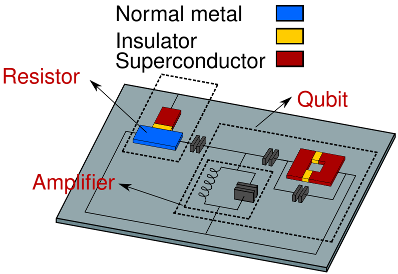
Evolution generates system-environment "entangled states"

$$\left.\begin{aligned} \imath\,\partial_t\psi(t) &= \mathbb{H}\,\psi(t) \\ \psi(0) &= \mathscr{s}_1 \otimes \mathscr{e}_1 \end{aligned}\right\} \Rightarrow \psi(t) = \sum_{i=1}^{\dim \mathscr{H}_S} \sum_{i=1}^{\dim \mathscr{H}_E} c_{i,j}(t)\, \mathscr{s}_i \otimes \mathscr{e}_j \neq \psi_S(t) \otimes \psi_E(t)$$

$\{\mathscr{s}_i\}_{i=1}^{\dim \mathscr{H}_S}$, $\{\mathscr{e}_i\}_{i=1}^{\dim \mathscr{H}_E}$ complete bases of $\mathscr{H}_S$, $\mathscr{H}_E$ resp.

Quantum Integrated circuit

- Qubit
- Amplifier (LC circuit)
- Resistor element: $\mathscr{N} = 10^9$ fermions



The distinctive trait

When two systems, of which we know the states by their respective representatives, enter into temporary physical interaction due to known forces between them, and when after a time of mutual influence the systems separate again, then they can no longer be described in the same way as before, viz. by endowing each of them with a representative of its own. I would not call that one but rather the characteristic trait of quantum mechanics, the one that enforces its entire departure from classical lines of thought. By the interaction the two representatives [the quantum states] have become entangled.

———————

Erwin Schrödinger

"Discussion of Probability Relations Between Separated Systems"

Proceedings of the Cambridge Philosophical Society, 1935

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The macroscopic objectification problem

Initial state: system + measurement device, tensor product

- Observable $\mathbb{A}$ of the system $\mathbb{A} = \sum_{i=1}^{d} a_i v_i v_i^{\dagger}$
- Initial state of the system $\psi_o = (v_1 + v_2)/\sqrt{2}$
- Measurement device: in a ready state $\mu_{\mathscr{r}}$ out of a set of $\{\mu_i\}_{i \geq 1}$ orthogonal states (i.e distinguishible macroscopic)

Final state: system + measurement device entangled

$$\mathbb{U}_t \psi \otimes \mu_{\mathscr{r}} = (v_1 \otimes \mu_1 + v_2 \otimes \mu_2)/\sqrt{2}$$

the apparatus is not in any macroscopic definite configuration!

A more general argument: Bassi and Ghirardi, *Physics Letters A*, (2000)

Dynamic postulate II (von Neumann-Pauli-Lüders)

The generalized measurement postulate

- An experiment has $\mathscr{M}$ distinct possible outcomes.
- To the i-th outcome is associated an operator $\mathbb{M}_i$ on $\mathscr{H}$ so that

$$\sum_{k=1}^{\mathscr{M}} \mathbb{M}_i^\dagger \mathbb{M}_i = \mathbb{1}_d \qquad d = \dim \mathscr{H}$$

- If the i-th outcome is observed, the state collapses to a new value

$$\psi(t) \to \psi'(t + \mathrm{d}t) = \frac{\mathbb{M}_i \psi(t)}{\|\mathbb{M}_i \psi(t)\|}$$

"Quantum Jumps"

Two dynamics?

We never experiment with just one electron or atom or (small) molecule. In thought-experiments we sometimes assume that we do; this invariably entails ridiculous consequences..

Erwin Schrödinger, "Are there Quantum Jumps?",
The British Journal for the Philosophy of Science, 1952.
As quoted in
Serge Haroche, and Jean-Michel Raimond,
"Exploring the Quantum: Atoms, Cavities, and Photons" Chap 1
Oxford Graduate Texts, 2006, X,616.

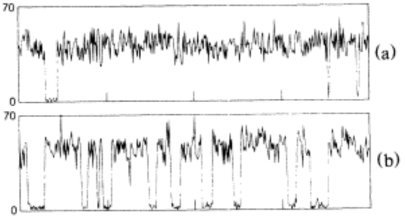
From "Neverwhere" to everywhere

VOLUME 57, NUMBER 14 PHYSICAL REVIEW LETTERS 6 OCTOBER 1986

Observation of Quantum Jumps in a Single Atom

J. C. Bergquist, Randall G. Hulet, Wayne M. Itano, and D. J. Wineland
Time and Frequency Division, National Bureau of Standards, Boulder, Colorado 80303
(Received 23 June 1986)

We detect the radiatively driven electric quadrupole transition to the metastable ${}^2D_{5/2}$ state in a single, laser-cooled Hg II ion by monitoring the abrupt cessation of the fluorescence signal from the laser-excited ${}^2S_{1/2} \rightarrow {}^2P_{1/2}$ first resonance line. When the ion "jumps" back from the metastable D state to the ground S state, the $S \rightarrow P$ resonance fluorescence signal immediately returns. The statistical properties of the quantum jumps are investigated; for example, photon antibunching in the emission from the D state is observed with 100% efficiency.



2012 Nobel Prize in Physics

Serge Haroche and David J. Wineland, for *ground-breaking experimental methods that enable measuring and manipulation of individual quantum systems*"

Wineland, *Reviews of Modern Physics*, (2013)

A lesson in life

Which goes to show that the best of us must sometimes eat our words,

———————

Albus P. W. B. Dumbledore
as quoted in
J.K. Rowlings
"Harry Potter and the Chamber of Secrets" Chap 18
Bloomsbury 1998.

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The GKLS master equation

Effective dynamics from the measurement postulate

Classical master equation

- A set $\{s_\alpha\}_{\alpha=1}^{d}$ of states.
- $w(i|j) = \text{Rate}(s_j \to s_i)$
- $\sum_{i \in \mathbb{I}} w(i|j) = 1$
- $\mathrm{p}(i,t)$ probability to find the system in the state s_i at time t before the transition.
- After transition

$$\mathrm{p}(i, t + \mathrm{d}t) = \sum_{j=1}^{d} w(i|j)\,\mathrm{p}(j,t)$$

Non selective measurement

- A set $\{\mathbb{M}_\alpha\}_{\alpha=1}^{\mathscr{M}}$ of operators.
- $\wp_\alpha = \text{Tr}\left(\mathbb{M}_\alpha\, \rho\, \mathbb{M}_\alpha^\dagger\right)$ probability of observing α if the state of the system is $\boldsymbol{\rho}$ **before** the measurement.
- $\sum_{\alpha=1}^{\mathscr{M}} \mathbb{M}_\alpha^\dagger \mathbb{M}_\alpha = \mathbb{1}_d$
- Selective measurement:

$$\rho_\alpha(t) = \frac{\mathbb{M}_\alpha \rho(t) \mathbb{M}_\alpha^\dagger}{\text{Tr}\left(\mathbb{M}_\alpha\, \rho(t)\, \mathbb{M}_\alpha^\dagger\right)}$$

- Non-selective measurement:

$$\rho'(t) = \sum_\alpha \wp_\alpha\, \rho_\alpha(t)$$

$$\rho(t + \mathrm{d}t) = \sum_\alpha \wp_\alpha \, \rho_\alpha(t) = \sum_\alpha \mathsf{M}_\alpha \rho(t) \mathsf{M}_\alpha^\dagger$$

- "Null outcome": for $\mathbb{H}^\dagger = \mathbb{H}$ and $\mathbb{R}^\dagger = \mathbb{R} = \mathbb{A}^\dagger \, \mathbb{A}$ (positive definite)

$$\mathbb{M}_0 = \mathbb{1}_d - \left(\imath \, \mathbb{H} + \frac{\mathbb{R}}{2} \right) \mathrm{d}t + o(\mathrm{d}t)$$

- "Jump" outcome: $\mathsf{M}_0^\dagger \mathsf{M}_0 = \mathbb{1} - \mathsf{M}_1^\dagger \mathsf{M}_1 + o(\mathrm{d}t)$ requires

$$\mathbb{M}_1 = \mathbb{A} \sqrt{\mathrm{d}t} + o(\sqrt{\mathrm{d}t})$$

Gorini-Kossakowski-Lindblad-Sudarshan (GKLS) equation

$$\rho(t + \mathrm{d}t) = \rho(t) - \left(\imath \, [\mathbb{H} \, , \rho(t)] + \frac{\mathbb{A}^\dagger \, \mathbb{A} \, \rho(t) + \rho(t) \, \mathbb{A}^\dagger \, \mathbb{A}}{2} - \mathbb{A} \, \rho(t) \, \mathbb{A}^\dagger \right) \mathrm{d}t$$

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Axiomatic rigorous derivation

Most general form always reducible to

$$\frac{\mathrm{d}}{\mathrm{d}t}\rho(t) = -\imath\,[\mathbb{H}\,,\rho(t)] - \sum_{\alpha=1}^{d^2-1}\left(\frac{\mathbb{L}_\alpha^\dagger\,\mathbb{L}_\alpha\,\rho(t) + \rho(t)\,\mathbb{L}_\alpha^\dagger\,\mathbb{L}_\alpha}{2} - \mathbb{L}_\alpha\,\rho(t)\,\mathbb{L}_\alpha^\dagger\right)$$

- Linear
- Markovian
- Self-adjoint
- Trace preserving: $\operatorname{Tr}\rho(t) = 1$
- Complete positivity

Sudarshan, Mathews, and Rau, *Physical Review*, (1961)

Lindblad, *Communications in Mathematical Physics*, (1976)

Gorini et al., *Journal of Mathematical Physics*, (1976)

A pedagogic derivation: Pearle, *European Journal of Physics*, (2012), ArXiv:1204.2016
History: Chruściński and Pascazio, *Open Systems & Information Dynamics*, (2017), ArXiv:1710.05993

The stochastic Schrödinger equation

Kolmogorov's picture of classical stochastic dynamics

Forward evolution of densities ("Schrödinger picture"):

$$\left.\begin{array}{l}(\partial_t + \partial_{\boldsymbol{x}} \cdot \boldsymbol{b}(\boldsymbol{x},t) - \operatorname{Tr} \partial_{\boldsymbol{x}} \otimes \partial_{\boldsymbol{x}} \mathbb{D}(\boldsymbol{x},t))\, p(\boldsymbol{x},t) = 0 \\ p(\boldsymbol{x},0) = p_o(\boldsymbol{x})\end{array}\right\} p(\boldsymbol{x},t) = \mathrm{E}\, \delta^d(\boldsymbol{\xi}_t - \boldsymbol{x})$$

Backward evolution of observables ("Heisenberg picture"):

$$\left.\begin{array}{l}(\partial_t + \boldsymbol{b}(\boldsymbol{x},t) \cdot \partial_{\boldsymbol{x}} + \operatorname{Tr} \mathbb{D}(\boldsymbol{x},t)\partial_{\boldsymbol{x}} \otimes \partial_{\boldsymbol{x}})\, f(\boldsymbol{x},t) = 0 \\ f(\boldsymbol{x},T) = f_o(\boldsymbol{x})\end{array}\right\} f(\boldsymbol{y},t) = \mathrm{E}\left(f_o(\boldsymbol{\xi}_T) \middle| \boldsymbol{\xi}_t = \boldsymbol{y}\right)$$

$$\begin{aligned} \mathrm{d}\boldsymbol{\xi}_t &= \boldsymbol{b}(\boldsymbol{\xi}_t,t)\mathrm{d}t + \sqrt{2\,\mathbb{D}}(\boldsymbol{\xi}_t,t)\mathrm{d}\boldsymbol{w}_t \\ \boldsymbol{\xi}_0 &\overset{\text{law}}{=} p_o \end{aligned} \qquad 0 \leq t \leq T$$

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"Unraveling" of the GKLS master equation

Evolution of state operators ("Schrödinger picture"):

$$\left.\begin{array}{l} \imath \dfrac{\mathrm{d}}{\mathrm{d}t}\rho(t) = [\mathbb{H}\,,\rho(t)] + \sum_{\alpha=1}^{d^2-1} \dfrac{[\mathbb{L}_\alpha^\dagger \mathbb{L}_\alpha\,,\rho(t)]_{+} - 2\mathbb{L}_\alpha\,\rho(t)\,\mathbb{L}_\alpha^\dagger}{2\,\imath} \\ \rho(0) = \rho_o \end{array}\right\} \quad \rho(t) = \mathrm{E}\,\psi_t\psi_t^\dagger$$

Evolution of observables ("Heisenberg picture"):

$$\frac{1}{\imath}\frac{\mathrm{d}}{\mathrm{d}t}\mathscr{X}(t) = [\mathbb{H}\,,\mathscr{X}(t)] - \sum_{\alpha=1}^{d^2-1} \frac{\mathbb{L}_\alpha^\dagger\mathbb{L}_\alpha\mathscr{X}(t) + \mathscr{X}(t)\mathbb{L}_\alpha^\dagger\mathbb{L}_\alpha - 2\mathbb{L}_\alpha^\dagger\,\mathscr{X}(t)\,\mathbb{L}_\alpha}{2\,\imath}$$

$$\mathscr{X}(t) = \mathrm{Tr}\left(\mathscr{X}\rho(t)\right) = \mathrm{E}\left(\psi_t^\dagger\mathbb{X}\psi_t\right)$$

$$\mathrm{d}\psi_t = \text{¿drift?}\,\mathrm{d}t + \text{¿diffusion?}\mathrm{d}\text{¿noise?}$$

$$\psi_0 \overset{\text{law}}{=} \rho_o$$

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Construction from the measurement postulate

To summarize:

- Measurement is a form of system-environment interaction.
- Incorporate the measurement into the dynamics

Working hypothesis: For given ψ the measurement only admits two outcomes:

- "Null result" with probability

$$\operatorname{Tr}\left(\psi(t)\psi^{\dagger}(t)\mathbb{M}_0^{\dagger}\mathbb{M}_0\right) = 1 - \operatorname{E}\left(\mathrm{d}\nu_t \middle| \psi(t)\right)$$

- "Detection" with (infinitesimally small) probability

$$\operatorname{Tr}\left(\psi(t)\psi^{\dagger}(t)\mathbb{M}_1^{\dagger}\mathbb{M}_1\right) = \operatorname{E}\left(\mathrm{d}\nu_t \middle| \psi(t)\right)$$

Detection occurs at random times $\Leftrightarrow$ increments of a Poisson process

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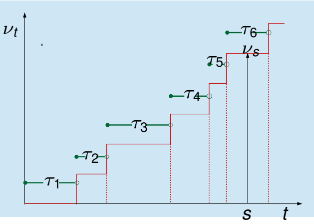
Quantum jump process

Poisson process $\{\nu_t\}_{t\geq 0}$:



independent increments

$$(\mathrm{d}\nu_t)^2 = \mathrm{d}\nu_t$$

$$\mathrm{E}\left(\mathrm{d}\nu_t|\psi(t)\right) = \|\mathbb{A}\boldsymbol{\psi}(t)\|^2\mathrm{d}t$$

$$\equiv \operatorname{Tr}\left(\psi(t)\psi^\dagger(t)\mathbb{M}_1^\dagger\mathbb{M}_1\right)$$

Measurements at random time induce the state's stochastic update rule

$$\boldsymbol{\psi}(t+\mathrm{d}t) = \boldsymbol{\psi}(t) + (1-\mathrm{d}\nu_t)\left(\frac{\mathbb{M}_0\boldsymbol{\psi}(t)}{\|\mathbb{M}_0\boldsymbol{\psi}(t)\|} - \boldsymbol{\psi}(t)\right) + \mathrm{d}\nu_t\left(\frac{\mathbb{A}\boldsymbol{\psi}(t)}{\|\mathbb{A}\boldsymbol{\psi}(t)\|} - \boldsymbol{\psi}(t)\right)$$

under the condition that <u>for all</u> $\psi(t)$

$$1 = \operatorname{Tr}\left(\psi(t)\psi^\dagger(t)\mathbb{M}_0^\dagger\mathbb{M}_0\right) + \operatorname{Tr}\left(\psi(t)\psi^\dagger(t)\mathbb{M}_1^\dagger\mathbb{M}_1\right)$$

$$\Rightarrow\ \mathbb{M}_0 = \mathbb{1}_d - \left(\imath\,\mathbb{H} + \frac{\mathbb{A}^\dagger\mathbb{A}}{2}\right)\mathrm{d}t + o(\mathrm{d}t)$$

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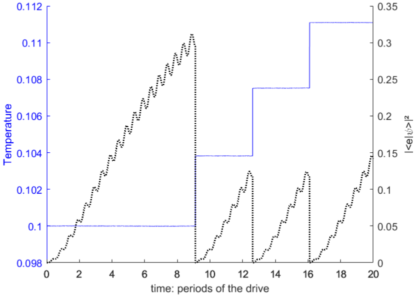
Stochastic Schrödinger equation I

Main result (after straightforward differential algebra):

$$d\psi(t) = -\left(\imath\mathbb{H} + \frac{\mathbb{A}^\dagger\,\mathbb{A}}{2} - \frac{\|\mathbb{A}\psi(t)\|^2}{2}\right)\psi(t)dt + \left(\frac{\mathbb{A}\psi(t)}{\|\mathbb{A}\psi(t)\|} - \psi(t)\right)d\nu_t$$

- Stochastic process in Ito sense: random increments independent of the current state of the system.
- Non-linear.
- Non-local.
- Pathwise probability preserving:

$$d\left(\psi^\dagger(t)\psi(t)\right) = 0$$



Dalibard, Castin, and Mölmer, *Physical Review Letters*, (1992)

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Stochastic Schrödinger equation II

Complex Wiener Noise

$$\mathrm{d}\psi(t) = -\left(\imath\mathbb{H} + \sum_{\alpha=1}^{d^2-1} \frac{\mathbb{L}_\alpha\mathbb{L}_\alpha + \psi^\dagger(t)\mathbb{L}_\alpha\psi(t)\mathbb{L}_\alpha - 2|\psi^\dagger(t)\mathbb{L}_\alpha\psi(t)|^2}{2}\right)\psi(t)\mathrm{d}t$$
$$+ \sum_{\alpha=1}^{d^2-1}\left(\mathbb{L}_\alpha - \psi^\dagger(t)\mathbb{L}_\alpha\psi(t)\right)\psi(t)\mathrm{d}\zeta_\alpha$$
$$\psi(0) = \psi_o$$

$$\mathrm{E}\,\mathrm{d}\zeta_\alpha = 0$$
$$\mathrm{E}\,\mathrm{d}\zeta_\alpha\zeta_\beta = 0$$
$$\mathrm{E}\,\mathrm{d}\zeta_\alpha^*\zeta_\beta = \delta_{a\,\beta}\mathrm{d}t$$

Gisin, *Physical Review Letters*, (1984)

Ghirardi, Rimini, and Weber, *Physical Review D*, (1986)

Gardiner, Parkins, and Zoller, *Physical Review A*, (1992)

I. C. Percival "*Quantum State Diffusion*" C U P 2003

Bassi and Ghirardi, *Physics Reports*, (2003)