Part I: On Sergey Vasilievich Vonsovsky (1910-1998)

The beginning: "Polar model"

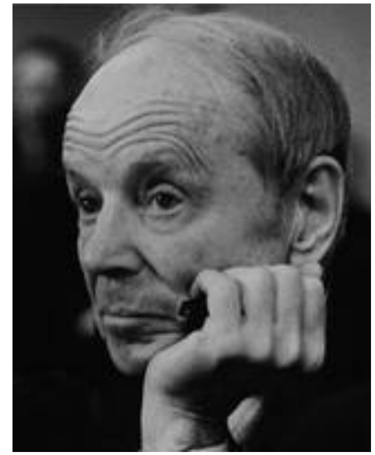
On the Electron Theory of Metals.

By S. Schubin and S. Wonsowsky.

Sverdlovsk Physical Technical Institute.

(Communicated by R. H. Fowler, F.R.S.—Received December 29, 1933.)

Proc. R. Soc. Lond. A 1934 **145**, published 2 June 1934



S. P. Shubin (1908-1938) S. V. Vonsovsky (1910-1998)

$$\int \frac{e^2}{|x - x'|} \phi_\alpha^2(x)\, \phi_\alpha^2(x')\, dx\, dx' = \mathrm{A}$$

$$\int \sum_{\gamma \neq \beta} \left[\mathrm{G}_\gamma(x)\, \phi_\alpha^2(x') + \frac{e^2}{|x - x'|} \phi_\gamma^2(x') \right] \phi_\alpha(x)\, \phi_\beta(x)\, dx\, dx' = \mathrm{L}_{\alpha\beta}$$

$$\int \frac{e^2}{|x - x'|} \phi_\alpha^2(x)\, \phi_\beta^2(x')\, dx\, dx' = \mathrm{B}_{\alpha\beta}$$

$$\int \frac{e^2}{|x - x'|} \phi_\alpha(x)\, \phi_\beta(x)\, \phi_\alpha(x')\, \phi_\beta(x')\, dx\, dx' = \mathrm{J}_{\alpha\beta}$$

Fig. 1.

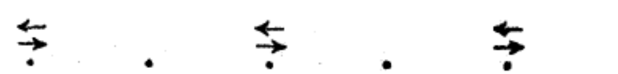


Fig. 2.

The beginning: "Polar model" II

Schrödinger equation in "atomic representation" (double *f*, hole *g*, spin right *k*, spin left *h*)

$$\{\varepsilon - s(\mathrm{A}+\mathrm{D}) - [\sum_{f<f'}(\mathrm{B}_{ff'} - \mathrm{J}_{ff'}) + \sum_{g<g'}(\mathrm{B}_{gg'} - \mathrm{J}_{gg'}) - \sum_{f,g}(\mathrm{B}_{fg} + \mathrm{J}_{fg})]\}\mathrm{C}(fgh)$$
$$+ \sum_{h,k}\mathrm{J}_{hk}[\mathrm{C}(\mathrm{T}_{hk}|fgh) - \mathrm{C}(fgh)] + \sum_{f,g}\mathrm{J}_{fg}[\mathrm{C}(\mathrm{T}_{fg}|fgh) - \mathrm{C}(fgh)]$$
$$+ \sum_{f,p}\mathrm{L}_{fp}\mathrm{C}(\mathrm{T}_{fp}|fgh) - \sum_{g,p}\mathrm{L}_{gp}\mathrm{C}(\mathrm{T}_{gp}|fgh) = 0, \quad (9)$$

Metal-insulator transition and Mott insulators

(II). The minimum energy corresponds to a certain $s = s_0$, where $0 < s_0 < n$. This case we have, for instance, when

$$\mathrm{A} + 6(\mathrm{J} - \mathrm{B}) > 0, \quad \mathrm{A} + 6\mathrm{J} - 12\mathrm{L} < 0.$$

Then, so long as s remains small, the lowest energy level *diminishes* as s increases; for a certain $s = s_0$ it attains a minimum and then again begins to increase. For such metals—at not very high temperatures—the number of "free" electrons approximates to twice this s_0 (electrons + holes!) and is therefore *smaller* than the number of atoms. In order to calculate s_0 in terms of our integrals, the energy must be evaluated up to the second approximation in powers of s/n; we shall not, however, make these rather cumbersome calculations here.

Metal

(III). The minimum energy corresponds to $s = 0$. This is the case when

$$\mathrm{A} + 6(\mathrm{J} - \mathrm{B}) > 0, \quad \mathrm{A} + 6\mathrm{J} - 12\mathrm{L} > 0.$$

Insulator

Quantum Hamiltonians: Lattice models I

For simplicity: single-band model

$$c_{i\sigma} = \sum_{\vec{k}} c_{\vec{k}\sigma} \exp\left(i\vec{k}\vec{R}_i\right),$$

From sites to bands:

$$c_{\vec{k}\sigma} = \sum_i c_{i\sigma} \exp\left(-i\vec{k}\vec{R}_i\right)$$

Band Hamiltonian

$$\hat{H}_0 = \sum_{\vec{k}\sigma} t_{\vec{k}} \hat{c}^+_{\vec{k}\sigma} \hat{c}_{\vec{k}\sigma}$$

$t_{\vec{k}}$ **is the Fourier transform of the hopping parameters** t_{ij}

Simple models: Hubbard model

$$\hat{H} = \sum_{ij\sigma}{}' t_{ij} \hat{c}^+_{i\sigma} \hat{c}_{j\sigma} + U \sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}$$

(only on-site Coulomb repulsion)

Extended Hubbard model
(intersite interactions added)

$$\hat{n}_{i\sigma} = \hat{c}^+_{i\sigma} \hat{c}_{i\sigma}, \qquad \hat{n}_i = \sum_\sigma \hat{n}_{i\sigma}$$

$$\hat{H}_c = U \sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow} + \frac{1}{2} \sum_{ij}{}' V_{ij} \hat{n}_i \hat{n}_j$$

Quantum Hamiltonians: s-d exchange model

s-d exchange (Vonsovsky-Zener) model: interaction of localized and itinerant electrons

$$\hat{H} = \sum_{ij\sigma}{}' t_{ij}\hat{c}^{+}_{i\sigma}\hat{c}_{j\sigma} - 2I\sum_{i}\hat{\vec{S}}_i\hat{\vec{s}}_i - \sum_{ij\sigma}{}' J_{ij}\hat{\vec{S}}_i\hat{\vec{S}}_j$$

The Hamiltonian written by Vonsovsky and Turov (1953)

Consequences: Kondo effect (!!!), RKKY (!!!), magnetic semiconductors…

One of the most important models in condensed matter theory

In particular: Cooper pairing via spin waves (Vonsovsky & Svirsky, 1960^{th})

1981: what to do next?

(1) The role of empty 3d states in Ca etc. (done, by Sasha Trefilov and me)
(2) Criterion of separation of electrons into core and itinerant (also, S.T. and me)
(3) The role of 6p electrons in rare earth - ???

Other problem: small itinerant FMs (around 1979)

PHYSICAL REVIEW B **84**, 045422 (2011)

Enhancement of the Curie temperature in small particles of weak itinerant ferromagnets

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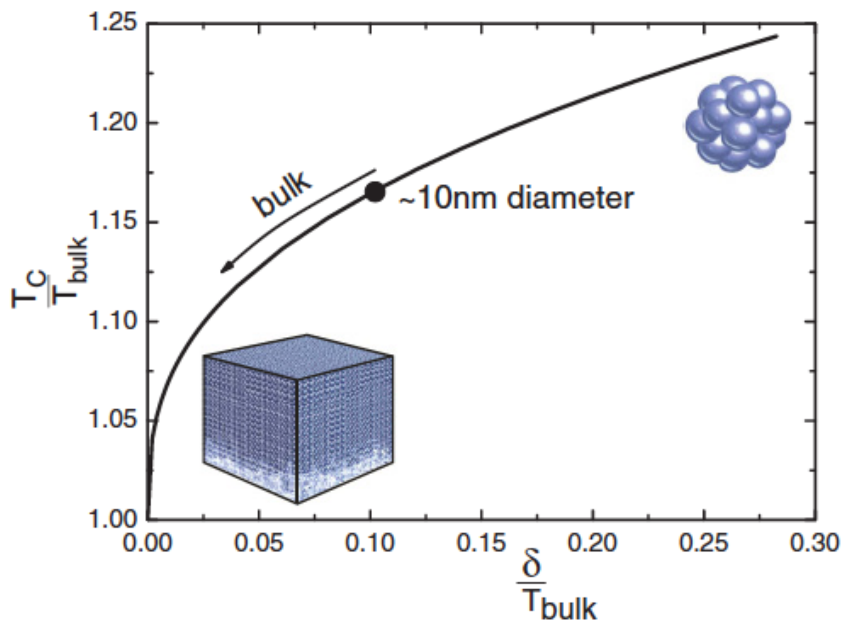
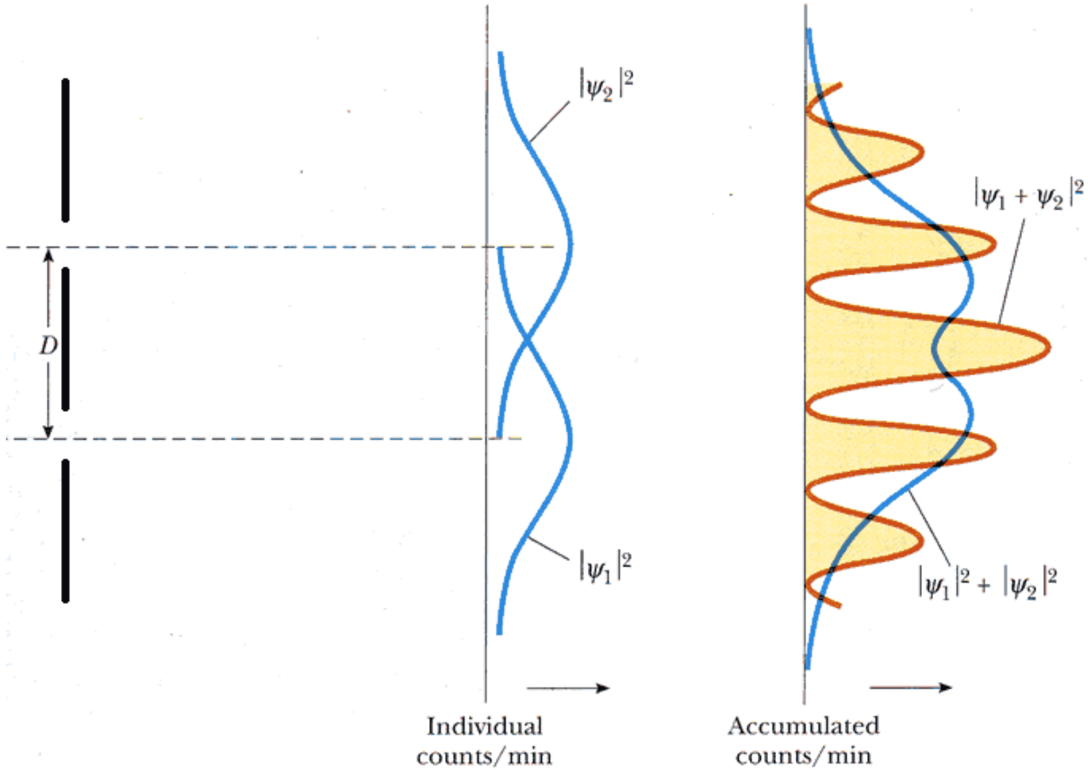
(Received 11 March 2011; revised manuscript received 13 May 2011; published 12 July 2011)



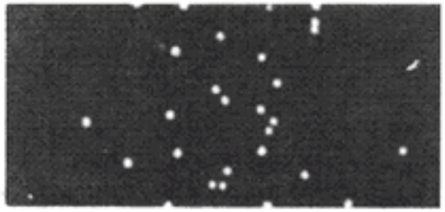
Part II: On measurement in quantum physics

Microworld: waves are corpuscles, corpuscles are waves

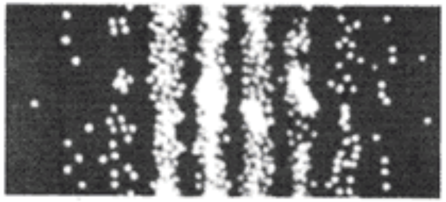
Einstein, 1905 – for light (photons)
L. de Broglie, 1924 – electrons and other microparticles



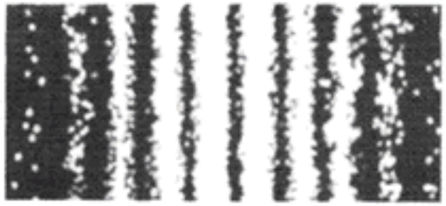
Electrons are particles (you cannot see half of electron) but moves along ***all*** possible directions (interference)



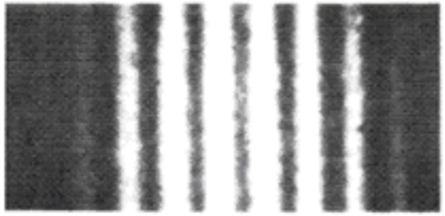
(a) After 28 electrons



(b) After 1000 electrons



(c) After 10000 electrons

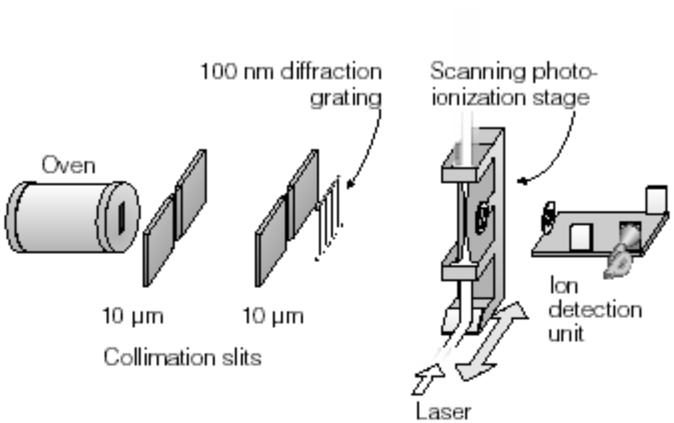


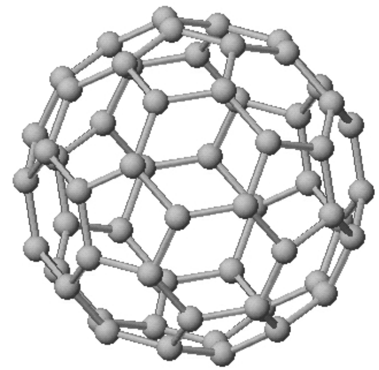
Universal property of matter

Wave–particle duality of C_{60} molecules

Markus Arndt, Olaf Nairz, Julian Vos-Andreae, Claudia Keller, Gerbrand van der Zouw & Anton Zeilinger

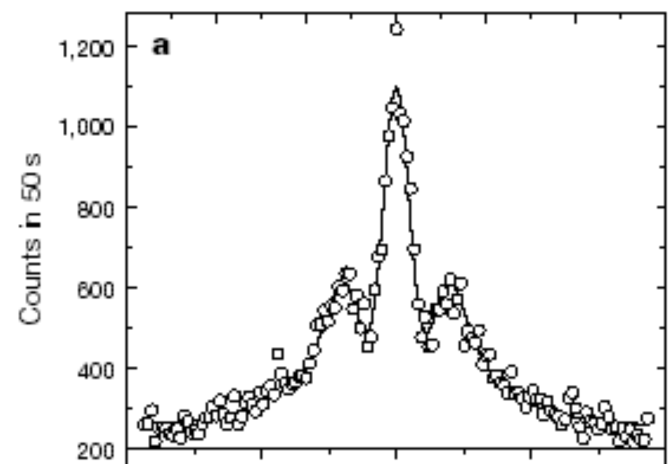
NATURE | VOL 401 | 14 OCTOBER 1999 |

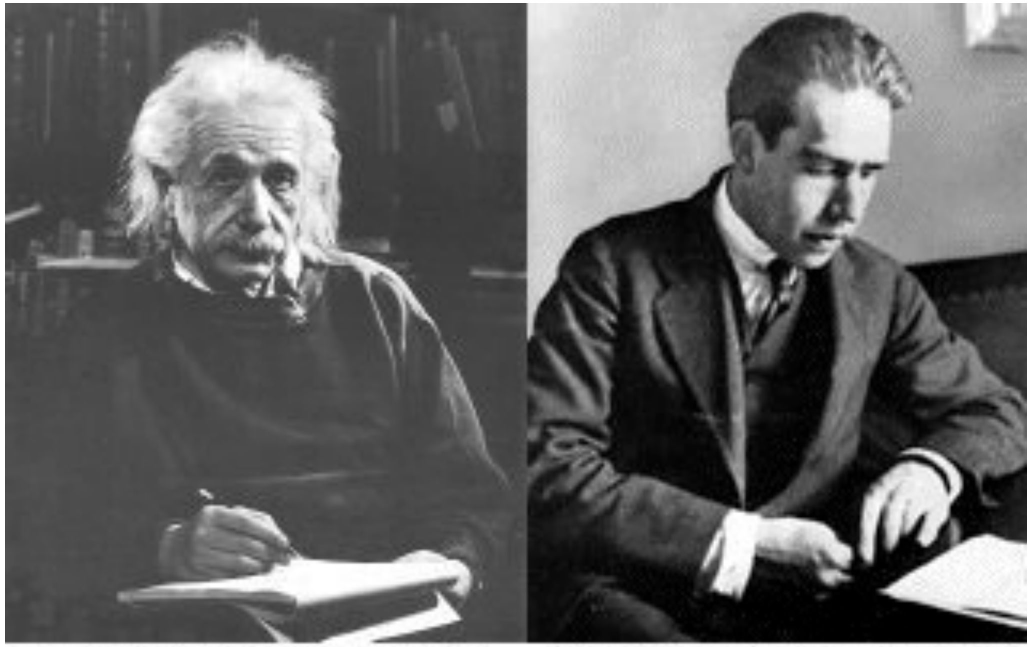




C_{60}

Matter waves for C_{60} molecules





God does not play dice with the universe. - Albert Einstein

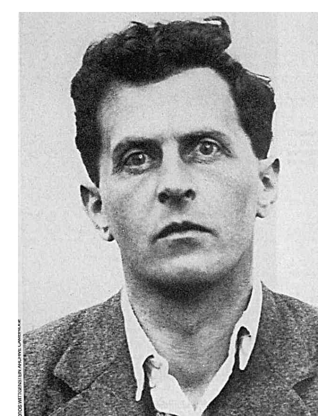
Anyone who is not shocked by Quantum Theory has not understood it. - Niels Bohr

A. Einstein: Quantum mechanics is incomplete; superposition principle does not work in the macroworld

N. Bohr: Classical measurement devices is an important part of quantum reality; we have to describe quantum world in terms of a language created for macroworld

The limits of my language mean the limits of my world

(Ludwig Wittgenstein)



Complementary principle: we live in classical world, our language is classical, we know nothing on the electron itself, we deal only with the results of its interaction with classical measuring devices

Classical physics is not just a limit of quantum physics at $\hbar \to 0$: we need classical objects!

(cf relativity theory: $c \to \infty$)

Used to be mainstream but now: quantum cosmology (no classical objects in early Universe)... quantum informatics ("as you can buy wavefunction in a supermarket")... Many-world interpretation...

I will be talking on quantum description of world around us

Von Neumann theory of measurement (1932)

Density matrix for subsystem A of a total system A + B

$$\rho(\alpha,\alpha') = Tr_\beta \Psi^*(\alpha',\beta)\Psi(\alpha,\beta)$$

$$\rho = \sum_a W_a |a\rangle\langle a|$$

Pure state $\rho = |a\rangle\langle a|$

$$\rho^2 = \rho$$

Mixed state $Tr\rho^2 < Tr\rho$

Two ways of evolution

1. Unitary evolution

$$i\hbar \frac{\partial \rho}{\partial t} = [H, \rho]$$

$$\rho(t) = \exp(iHt/\hbar)\rho(0)\exp(-iHt/\hbar)$$

Entropy is conserved

$$S = -Tr\rho \ln \rho$$

2. Nonequilibrium evolution by the measurement

$$\rho_{after} = \sum_n P_n \rho_{before} P_n$$

$$P_n = |n\rangle\langle n|$$

$$S_{after} > S_{before}$$

Density matrix after the measurement is diagonal in n-representation

Application: decoherence wave

PHYSICAL REVIEW A, VOLUME 62, 022118

Propagation of local decohering action in distributed quantum systems

M. I. Katsnelson,* V. V. Dobrovitski, and B. N. Harmon

PHYSICAL REVIEW B, VOLUME 63, 212404

Néel state of an antiferromagnet as a result of a local measurement in the distributed quantum system

M. I. Katsnelson,* V. V. Dobrovitski, and B. N. Harmon

Example: Bose-Einstein condensation in ideal and almost ideal gases

$$H=\sum_{\mu} E_{\mu}\alpha_{\mu}^{\dagger}\alpha_{\mu} \qquad |\Psi\rangle=\frac{1}{\sqrt{M!}}(\alpha_0^{\dagger})^{M}|0\rangle$$

0 is the state with minimal energy

We measure at $t = 0$ number of bosons at a given lattice site

Projection operator:

$$W_n=\delta_{n,N}=\int_0^{2\pi}\frac{d\phi}{2\pi}\exp[i\phi(n-N)]$$

Von Neumann prescription:

$$U(t)=\sum_{n=0}^{\infty} \exp(-iHt)W_n U_{\rm in}W_n^{\dagger}\exp(iHt)$$

$U_{\rm in}=|\Psi\rangle\langle\Psi|$ is the density matrix before measurement

Decoherence wave in BEC

Single-particle density matrix $\rho(\mathbf{r},\mathbf{r}',t) = \mathrm{Tr}[U(t)a^\dagger(\mathbf{r}')a(\mathbf{r})]$

Explicit calculations

Poisson statistics for the measurement outcomes

$$p_n = e^{-n_0} n_0^n/(n!) \qquad n_0 = n_B(0)$$

$$S = -\mathrm{Tr}[U(t)\ln U(t)] = -\sum_{n=0}^{\infty} p_n \ln p_n > 0$$

$$\rho(\mathbf{r},\mathbf{r}',t) = \sqrt{n_B(\mathbf{r})n_B(\mathbf{r}')} - G^*(\mathbf{r}',t)\sqrt{n_B(\mathbf{r})n_0} - G(\mathbf{r},t)\sqrt{n_B(\mathbf{r}')n_0} + 2n_0 G^*(\mathbf{r}',t)G(\mathbf{r},t)$$

$$G(\mathbf{r},t) = V_0\left(\frac{m}{2\pi i\hbar t}\right)^{3/2}\exp\left(\frac{im\mathbf{r}^2}{2\pi\hbar t}\right)$$

$$\rho(\mathbf{r},\mathbf{r},t) = n_B + 2n_B V_0^2\left(\frac{m}{2\pi\hbar t}\right)^3 - 2n_B V_0\left(\frac{m}{2\pi\hbar t}\right)^{3/2}\cos\left(\frac{m\mathbf{r}^2}{2\pi\hbar t}\right)$$

Decoherence wave in BEC II

Weakly nonideal gas: Bogoliubov transformation

$$H=\sum_{\mathbf{k}} E_{\mathbf{k}}\alpha^{\dagger}_{\mathbf{k}}\alpha_{\mathbf{k}}$$

$$+\frac{1}{2V}\sum_{\mathbf{k}_1+\mathbf{k}_2=\mathbf{k}_1'+\mathbf{k}_2'} v(\mathbf{k}_1-\mathbf{k}_1')\alpha^{\dagger}_{\mathbf{k}_1'}\alpha^{\dagger}_{\mathbf{k}_2'}\alpha_{\mathbf{k}_2}\alpha_{\mathbf{k}_1}$$

$$\alpha_{\mathbf{k}}=\xi_{\mathbf{k}}\cosh\chi_{\mathbf{k}}+\xi^{\dagger}_{-\mathbf{k}}\sinh\chi_{\mathbf{k}},$$

$$\alpha^{\dagger}_{-\mathbf{k}}=\xi_{\mathbf{k}}\sinh\chi_{\mathbf{k}}+\xi^{\dagger}_{-\mathbf{k}}\cosh\chi_{\mathbf{k}},$$

$$\tanh 2\chi_{\mathbf{k}}=-\frac{v(\mathbf{k})n_B}{E_{\mathbf{k}}+v(\mathbf{k})n_B}$$

Excitation spectrum $\quad \omega_{\mathbf{k}}=\sqrt{E_{\mathbf{k}}^2+2E_{\mathbf{k}}v(\mathbf{k})n_B}.$

$$\rho_n(\mathbf{r},\mathbf{r}',t)=\frac{n_B}{(n!)^2}\frac{\partial^{2n}}{\partial z^n\partial z'^n}\{[1+(z-1)G(\mathbf{r},t)]$$

$$\times[1+(z'-1)G^*(\mathbf{r}',t)]$$

$$\times\exp[n_B X(z,z')]\}_{z=z'=0},$$

Acoustic for small *k*

$$X(z,z')=B(zz'-1)+(1-B)(z+z'-2)$$

$$+A[(z-1)^2+(z'-1)^2],$$

$$A=\frac{V_0}{2V}\sum_{\mathbf{k}}\frac{v(\mathbf{k})n_B}{\omega_{\mathbf{k}}},$$

$$B=\frac{V_0}{2V}\sum_{\mathbf{k}}\left[1+\frac{E_{\mathbf{k}}+v(\mathbf{k})n_B}{\omega_{\mathbf{k}}}\right],$$

$$G(\mathbf{r},t)=\sum_{\mathbf{k}}\exp(i\mathbf{k}\cdot\mathbf{r})\left\{\cos\omega_{\mathbf{k}}t-i\frac{E_{\mathbf{k}}+v(\mathbf{k})n_B}{\omega_{\mathbf{k}}}\sin\omega_{\mathbf{k}}t\right\}$$

Decoherence wave in BEC III

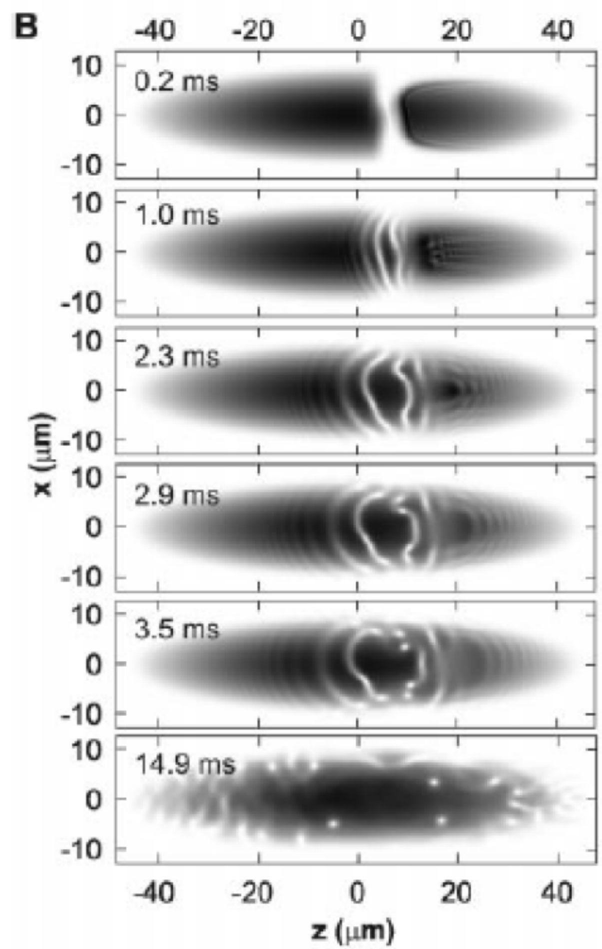
In this case, decoherent action propagates with sound velocity, nothing is “superluminal”, etc – a smooth “wave function collapse”

Can be experimentally verified! But, in a sense...

Observation of Quantum Shock Waves Created with Ultra-Compressed Slow Light Pulses in a Bose-Einstein Condensate

Zachary Dutton,[1,2] Michael Budde,[1,3] Christopher Slowe,[1,2] Lene Vestergaard Hau[1,2,3]

SCIENCE VOL 293 27 JULY 2001 663



Interaction with light is a measurement!

Neel state of AFM: The role of entanglement

$$\mathcal{H}_0 = \sum_{\mathbf{q}} J_{\mathbf{q}} (S_{\mathbf{q}}^+ S_{\mathbf{q}}^- + S_{\mathbf{q}}^z S_{\mathbf{q}}^z)$$

Ground state is singlet, no sublattices!

$$\sum_{\mathbf{q}} J_{\mathbf{q}} = 0, \qquad \min_{\mathbf{q}} J_{\mathbf{q}} = J_{\kappa}$$

Anomalous averages:

$$H \to H - hA$$

$$\lim_{h\to 0} \lim_{N\to\infty} \langle A \rangle \neq \lim_{N\to\infty} \lim_{h\to 0} \langle A \rangle$$

In the case of AFM (or superconductor) this field does not look physical!

On the Description of the Antiferromagnetism without Anomalous Averages

V.Yu. Irkhin and M.I. Katsnelson

Z. Phys. B – Condensed Matter 62, 201–205 (1986)

$$|\Phi_M\rangle \equiv |M\rangle = (S_{-\kappa}^-)^M |F\rangle$$

$$|\Phi\rangle = \sum_{L=0}^{NS} \exp[\lambda(L)/2] |2L\rangle$$

$|F\rangle$ is the ferromagnetic state (all spins up)

In thermodynamic limit, this state (without anomalous averages!) gives the same results for observables as Neel state; can be used as starting point for local measurement and decoherence wave

ON THE GROUND-STATE WAVEFUNCTION OF A SUPERCONDUCTOR IN THE BCS MODEL

V.Yu. IRKHIN and M.I. KATSNELSON

Volume 104A, number 3 PHYSICS LETTERS 20 August 1984

Neel state of AFM: The role of entanglement II

Measuring local spin at site n = 0

Easy-axis anisotropy: in Ising limit, one single measurement leads to instans wave function collapse: all even spins up, all odd down (or vice versa)

Easy plane anisotropy (or isotropic case) – broken continuous symmetry; Decoherence wave and of the order of *N* measurements to create Neel state

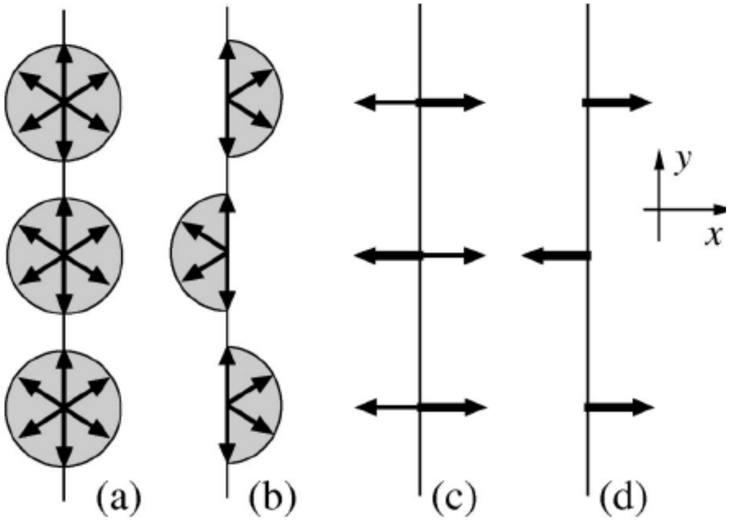


FIG. 1. Sketch of the spin arrangement. Easy plane case: (a) before measurement, sublattices are absent and the total AFM axis is not fixed; (b) after measurement, the "fan" sublattices emerge but an AFM axis is not fixed. Easy axis case: (c) before measurement, sublattices are absent; (d) after measurement, the Néel state appears.

However... This is for classical spins!

In AFM, there are zero-point oscillations: nominal spin is less than in classical Neel picture. E.g., square lattice Heisenberg AFM, NN interactions only:

$$\overline{S_0} = S - 0.1971$$

It means that for S=1/2 if a spin belongs to (nominally) spin-up sublattice in reality it is up with 80% probability and down with 20% probability (average spin is roughly 0.3)

Than, even in easy-axis case one single local measurement is not enough to establish sublattices – may be by accident it is done in a “wrong” instant

Decoherence waves in AFM for quantum spins

PHYSICAL REVIEW B **93**, 184426 (2016)

Decoherence wave in magnetic systems and creation of Néel antiferromagnetic state by measurement

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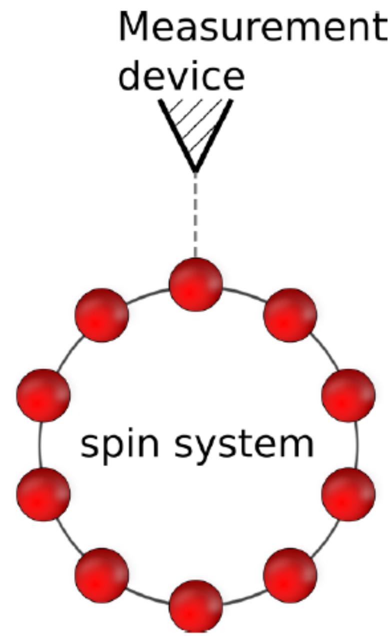
(Received 15 February 2016; published 20 May 2016)



Simulations by numerically exact solution of time-dependent Schrödinger equation

$$\rho \to \rho' = \textstyle\sum_i P_i \rho P_i \qquad P_m^{\pm\alpha} = \frac{1 \pm 2S_m^\alpha}{2} \qquad \langle S_l^\beta(t)\rangle = \mathrm{Tr}\left[S_l^\beta(t) \frac{P_m^{\pm\alpha}\rho_0 P_m^{\pm\alpha}}{N_0} \right]$$

Hamiltonian is the sum of Heisenberg and Ising parts:

$$H_0 = J \sum_{\langle i,j\rangle} \mathbf{S}_i \cdot \mathbf{S}_j \qquad H' = J\Delta \sum_{\langle i,j\rangle} S_i^z S_j^z$$

The larger Δ, the weaker are quantum zero-point oscillations

Chebyshev Polynomial Algorithm

Chebyshev Polynomial Algorithm: based on the numerically exact polynomial decomposition of the time evolution operator Ũ. It is very efficient if *H* is a sparse matrix.

$$\left|\varphi(t)\right\rangle = \widetilde{U}\left|\varphi(0)\right\rangle = e^{-itH}\left|\varphi(0)\right\rangle$$

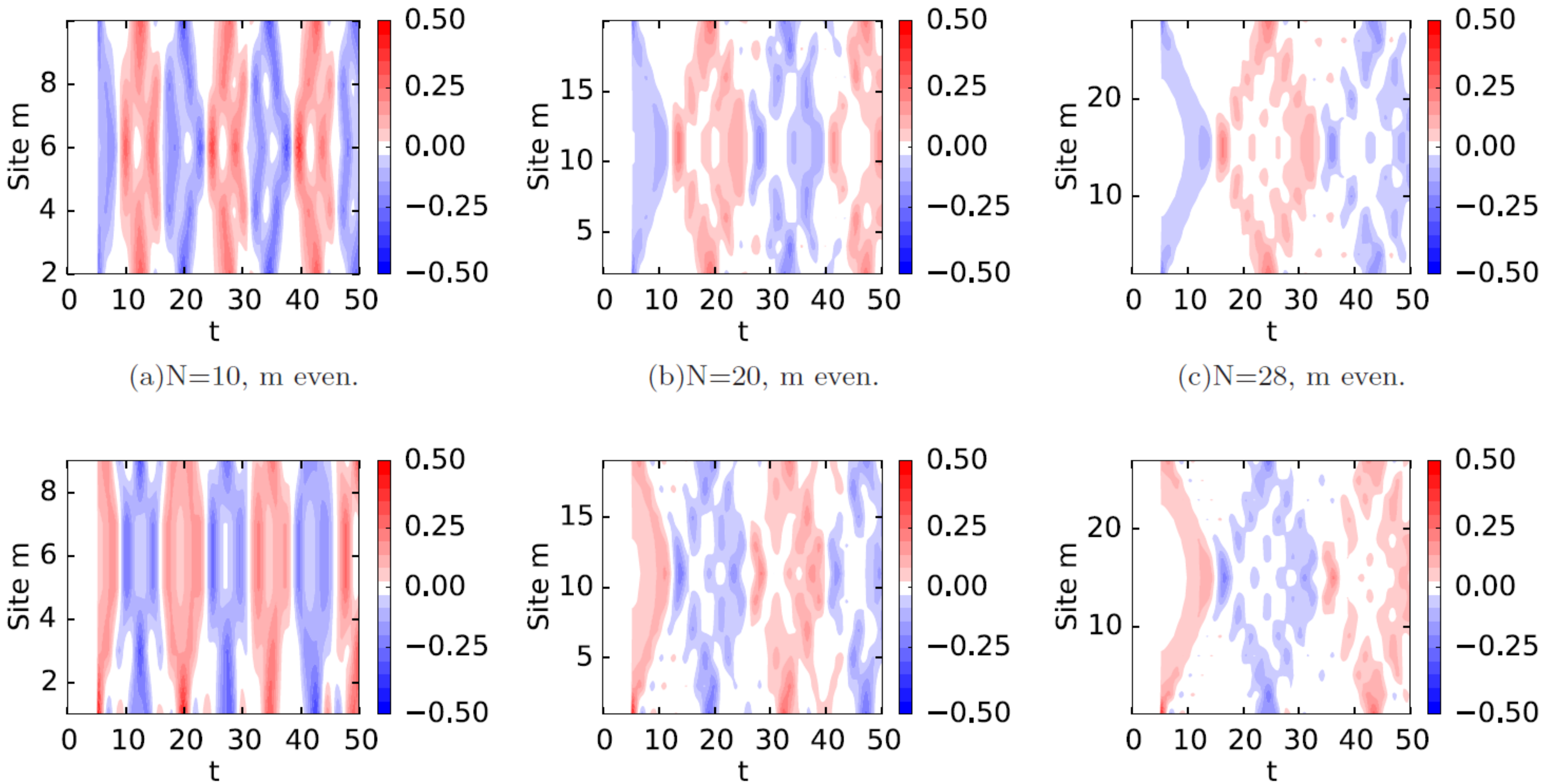
$$e^{-izx} = J_0(z) + 2\sum_{m=1}^{\infty}(-i)^m J_m(z) T_m(x)$$

$$T_m(x) = \cos[m\arccos(x)], x \in [-1,1]$$

$$T_{m+1}(x) + T_{m-1}(x) = 2xT_m(x)$$

Decoherence waves in AFM for quantum spins III

Single measurement



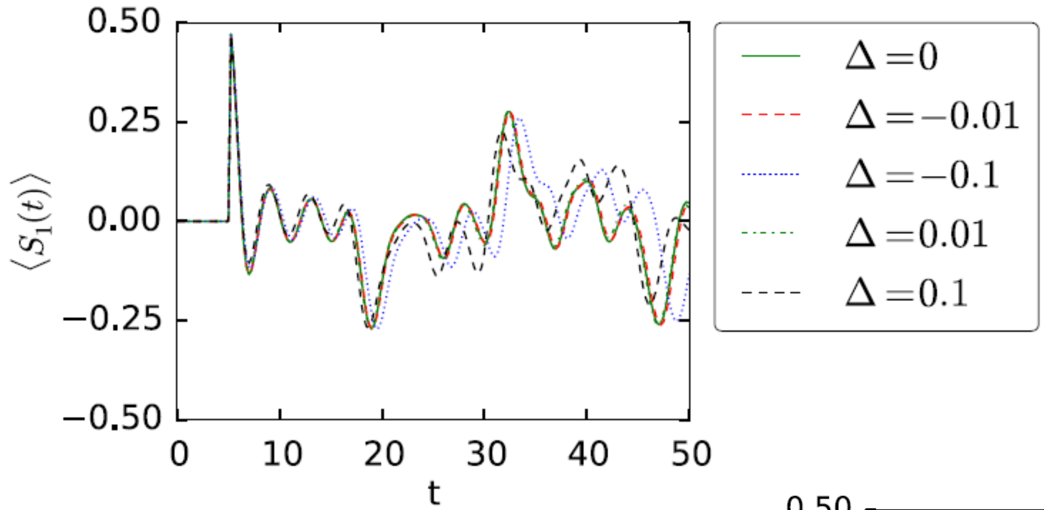
(a)N=10, m even. (b)N=20, m even. (c)N=28, m even.

(d)N=10, m odd. (e)N=20, m odd. (f)N=28, m odd.

FIG. 3. Time evolution of the magnetization $\langle S^z_m(t)\rangle$ for the isotropic (i.e., XXX) AFM Heisenberg spin chain of length N. The system at $t = 0$ is prepared in the ground state after which at $t = 5$ spin 1 is projected on the $+z$ axis.

Decoherence waves in AFM for quantum spins IV

The sign of anisotropy is not important if it is small



Also, multiple measurements were studied

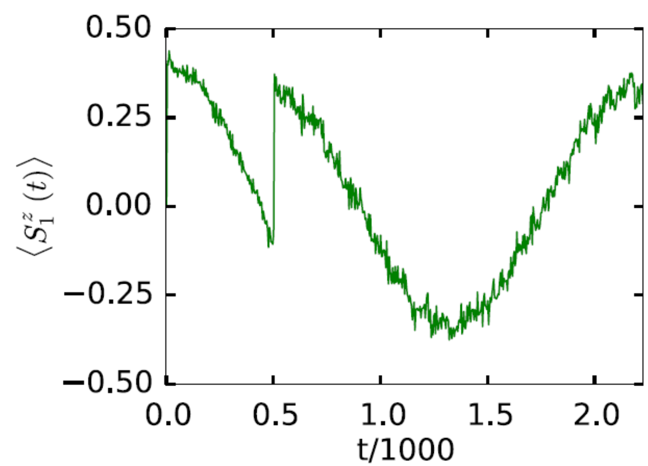
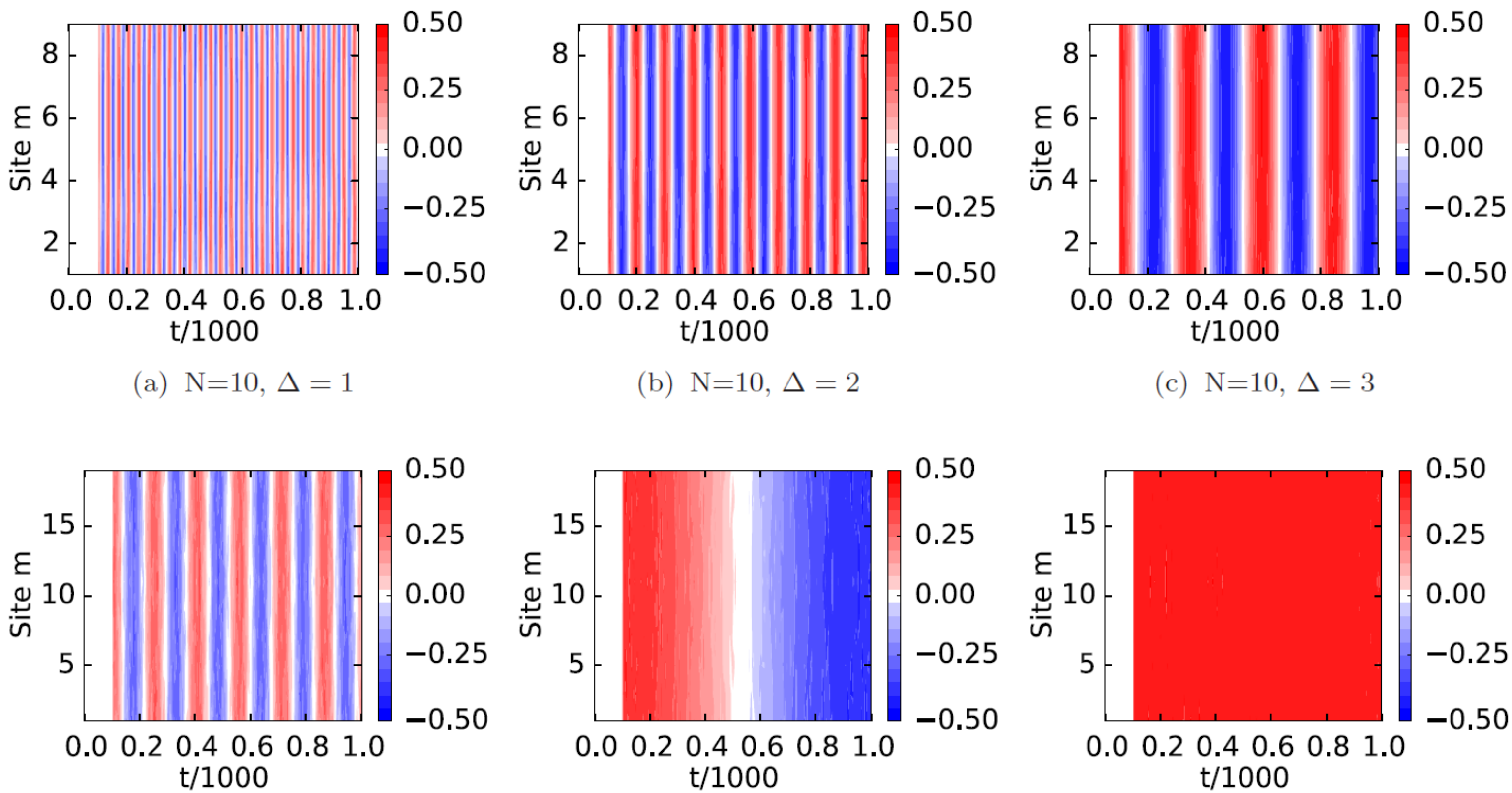


FIG. 7. Magnetization $\langle S_1^z \rangle$ for $N = 20$ and $\Delta = 2$, projections P_1^z are performed at $t = 1$ and $t = 500$. The subsequent measurement (at $t = 500$) restores the sublattice order (close) to the state after the first measurement.

Decoherence waves in AFM for quantum spins V

Oscillations of total magnetization after single local measurement



(a) N=10, $\Delta = 1$ (b) N=10, $\Delta = 2$ (c) N=10, $\Delta = 3$

(d) N=20, $\Delta = 1$ (e) N=20, $\Delta = 2$ (f) N=20, $\Delta = 3$

FIG. 9. Magnetization $\langle S_m^z \rangle$ for odd values of m for different values of the anisotropy Δ and chain length N. At $t = 0$, the system is prepared in the ground state, and at $t = 100$ a single measurement is performed on spin 1 along the z direction.

Direct attempts to simulate measurement as interaction with measuring device plus decoherence by environment

Quantum dynamics of a small symmetry breaking measurement device

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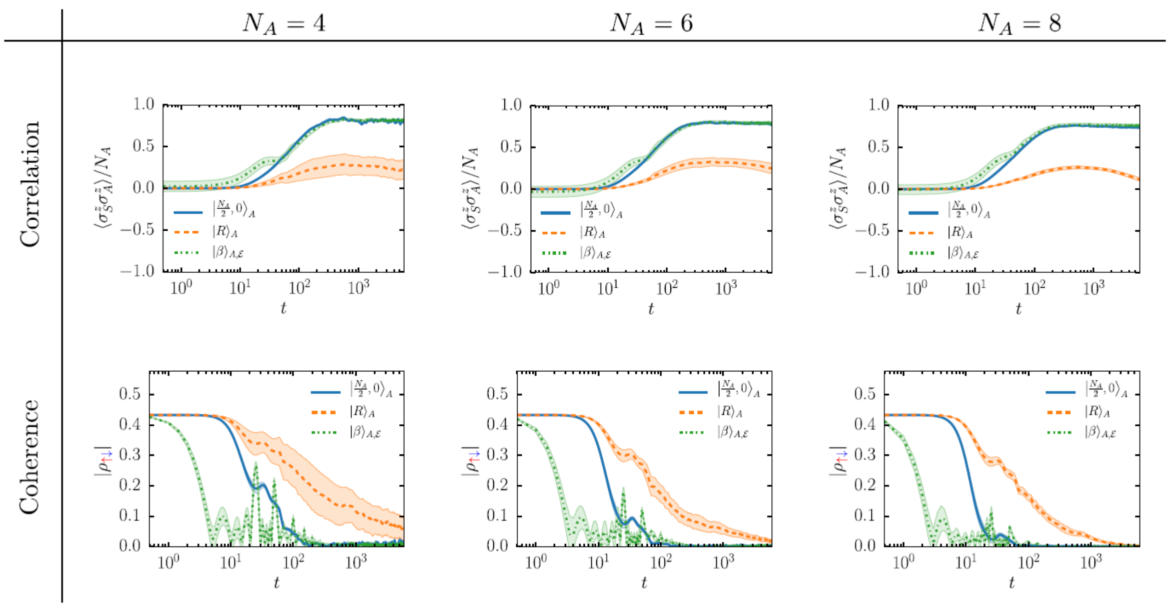
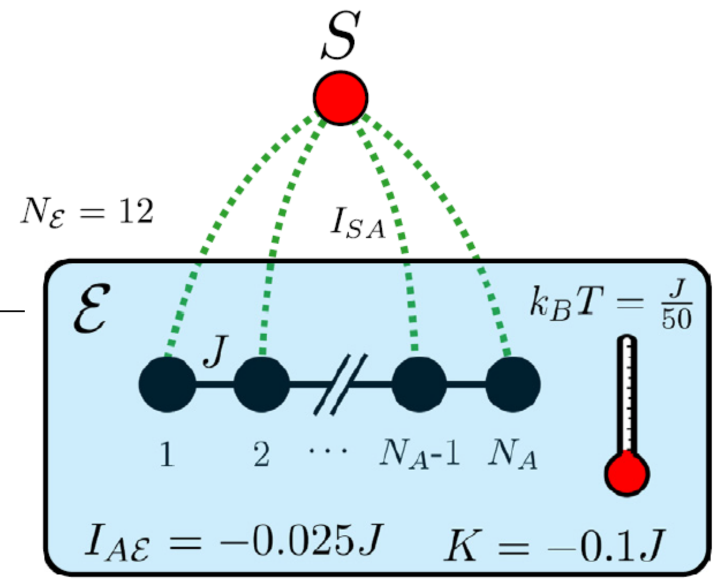
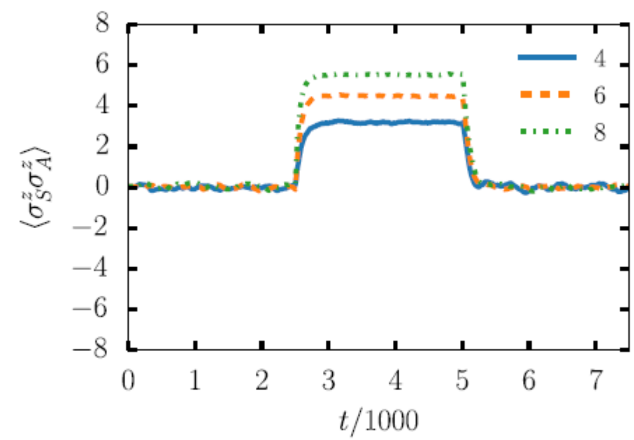
Annals of Physics 396 (2018) 137–146







Decay off-diagonal elements of density matrix - yes

Stability test – no stability

Radboud Universiteit

Does God play dice?

Mikhail Katsnelson

Collaborators

Hans De Raedt, RUG

Kristel Michielsen, Julich

Dennis Willsch, Julich

Hylke Donker, RU

LI approach - References

Quantum theory as the most robust description of reproducible experiments

Annals of Physics 347 (2014) 45–73

Hans De Raedt[a], Mikhail I. Katsnelson[b], Kristel Michielsen[c,d,*]

Quantum theory as a description of robust experiments: Derivation of the Pauli equation

Annals of Physics 359 (2015) 166–186

Hans De Raedt[a], Mikhail I. Katsnelson[b], Hylke C. Donker[b], Kristel Michielsen[c,d,*]

Logical inference approach to relativistic quantum mechanics: Derivation of the Klein–Gordon equation

Annals of Physics 372 (2016) 74–82

H.C. Donker[a,*], M.I. Katsnelson[a], H. De Raedt[b], K. Michielsen[c]

Logical inference derivation of the quantum theoretical description of Stern–Gerlach and Einstein–Podolsky–Rosen–Bohm experiments

Annals of Physics 396 (2018) 96–118

Hans De Raedt[a], Mikhail I. Katsnelson[b], Kristel Michielsen[c,d,*]

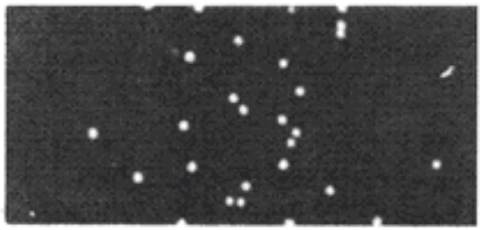
Quantum theory as plausible reasoning applied to data obtained by robust experiments

H. De Raedt[1], M. I. Katsnelson[2] and K. Michielsen[3,4]

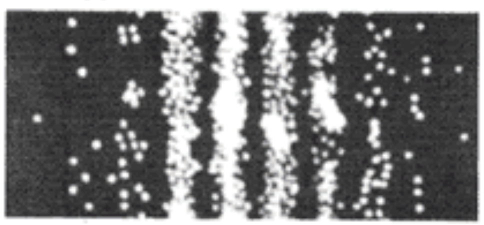
PHILOSOPHICAL TRANSACTIONS A

Cite this article: De Raedt H, Katsnelson MI, Michielsen K. 2016 Quantum theory as plausible reasoning applied to data obtained by robust experiments. *Phil. Trans. R. Soc. A* **374**: 20150233.

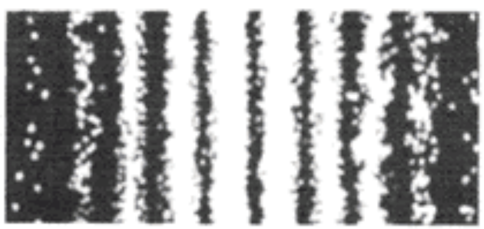
Electrons are particles (you cannot see half of electron) but moves along ***all*** possible directions (interference)



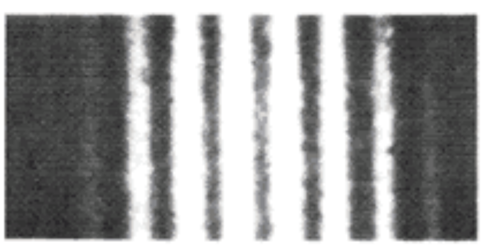
(a) After 28 electrons



(b) After 1000 electrons



(c) After 10000 electrons



We cannot describe individual events, individual spots seem to be completely random, but ensemble of the spots forms regular interference fridges

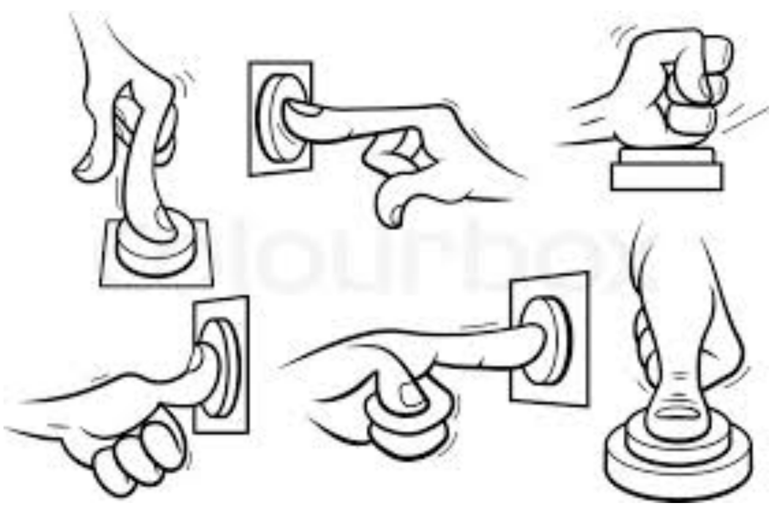
Randomness in the foundations of physics?!

Two ways of thinking

I. Reductionism ("microscopic" approach)

Everything is from water/fire/earth/gauge fields/quantum space-time foam/strings... and the rest is your problem

II. Phenomenology: operating with "black boxes"



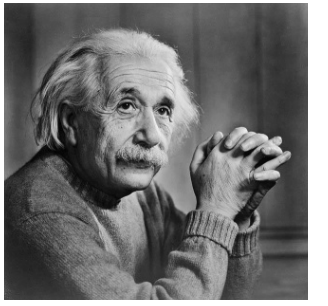
Two ways of thinking II

Knowledge begins, so to speak, in the middle, and leads into the unknown - both when moving upward, and when there is a downward movement. Our goal is to gradually dissipate the darkness in both directions, and the absolute foundation - this huge elephant carrying on his mighty back the tower of truth - it exists only in a fairy tales (Hermann Weyl)

We never know the foundations! How can we have a reliable knowledge without the base?

Is fundamental physics fundamental?

Classical thermodynamics is the only physical theory of universal content which I am convinced will never be overthrown, within the framework of applicability of its basic concepts (A. Einstein)



The laws describing our level of reality are essentially independent on the background laws. I wish our colleagues from *true* theory (strings, quantum gravity, etc....) all kind of success but either they will modify electrodynamics and quantum mechanics at atomic scale (and then they will be wrong) or they will not (and then I do not care). Our way is *down*

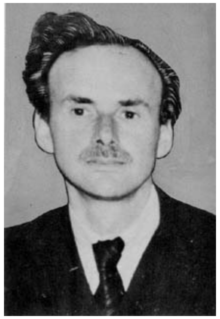
But how can we be sure that we are right?!

Mathematics & Physics

Newton: It is useful to solve (ordinary) differential equations

Maxwell: It is useful to solve *partial* differential equations

Heisenberg, Dirac, von Neumann et al: It is useful to consider state vectors and operators in Hilbert space



But this is much farther from usual human intuition – may be, too far?!

Can we demistify it?!

Unreasonable effectiveness

- Quantum theory describes a vast number of different experiments very well

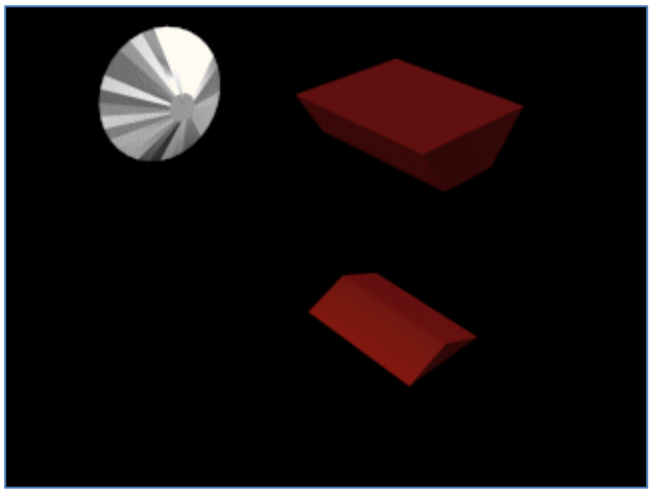
- WHY ?

- Niels Bohr*:
  It is wrong to think that the task of physics is to find out how nature *is*.
  Physics concerns what we can *say* about nature.

*A. Petersen, "The philosophy of Niels Bohr," Bulletin of the Atomic Scientists 19, 8 – 14 (1963).

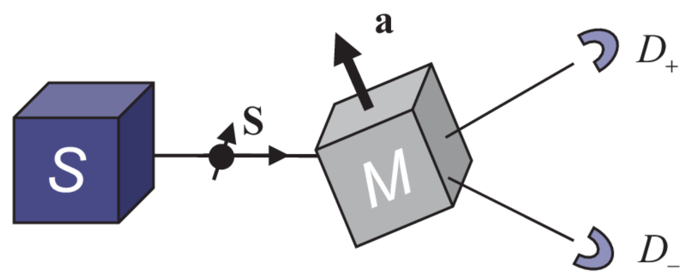
Stern-Gerlach experiment

- Neutral atoms (or neutrons) pass through an inhomogeneous magnetic field



- Inference from the data: directional quantization

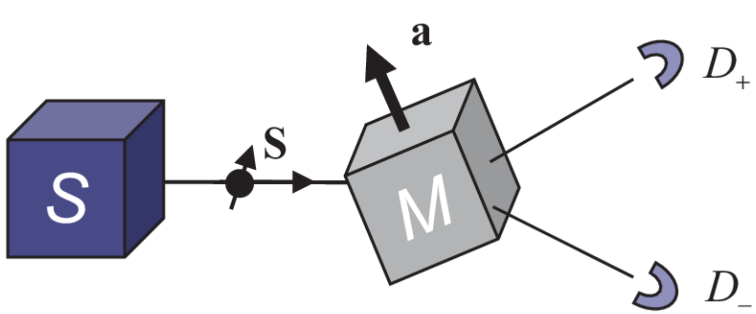
- Idealization



- Source *S* emits particles with magnetic moment
- Magnet *M* sends particle to one of two detectors
- Detectors count every particle

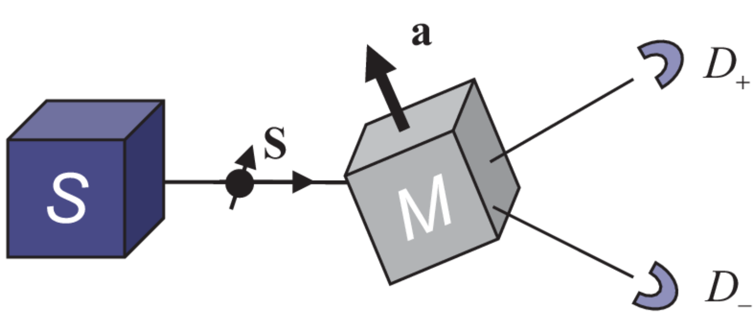
Some reasonable assumptions (1)

- For fixed **a** and fixed source *S*, the frequencies of + and – events are reproducible
- If we rotate the source *S* and the magnet *M* by the same amount, these frequencies do not change

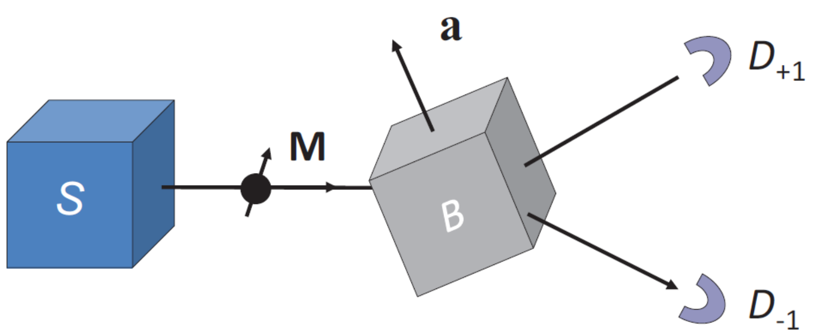


Some reasonable assumptions (2)

- These frequencies are robust with respect to small changes in **a**
- Based on all other events, it is impossible to say with some certainty what the particular event will be (logical independence)



Logical inference



- Shorthand for propositions
  - x=+1 ⇔ D_+ clicks
  - x=-1 ⇔ D_- clicks
  - **M** ⇔the value of **M** is **M**
  - **a** ⇔the value of **a** is **a**
  - **Z** ⇔everything else which is known to be relevant to the experiment but is considered to fixed
- We assign a real number $P(x|\mathbf{M},\mathbf{a},Z)$ between 0 and 1 to express our expectation that detector D_+ or (exclusive) D_- will click and want to derive, not postulate, $P(x|\mathbf{M},\mathbf{a},Z)$ from general principles of rational reasoning
- What are these general principles ?

Plausible, rational reasoning ➔ inductive logic, logical inference

- G. Pólya, R.T. Cox, E.T. Jaynes, …
  - From general considerations about rational reasoning it follows that the plausibility that a proposition *A* (*B*) is true given that proposition *Z* is true may be encoded in real numbers which satisfy

$$0 \leq P(A|Z) \leq 1$$

$$P(A|Z) + P(\bar{A}|Z) = 1 \quad ; \quad \bar{A} = \text{NOT } A$$

$$P(AB|Z) = P(A|BZ)P(B|Z) \quad ; \quad AB = A \text{ AND } B$$

  - Extension of Boolean logic, applicable to situations in which there is uncertainty about some but not all aspects
    - Kolmogorov’s probability theory is an example which complies with the rules of rational reasoning
    - Is quantum theory another example?

Plausible, rational reasoning ➔ logical inference II

- Plausibility
  - Is an intermediate mental construct to carry out inductive logic, rational reasoning, logical inference
  - May express a degree of believe (subjective)
  - May be used to describe phenomena independent of individual subjective judgment

    plausibility ➔ i-prob (inference-probability)

Application to the Stern-Gerlach experiment

We repeat the experiment N times. The number of times that D_+ (D_-) clicks is n_+ (n_-)

i-prob for the individual event is

$$P(x|\mathbf{a}\cdot\mathbf{M},Z)=P(x|\theta,Z)=\frac{1+xE(\theta)}{2} \quad , \quad E(\theta)=E(\mathbf{a}\cdot\mathbf{M},Z)=\sum_{x=\pm1}xP(x|\theta,Z)$$

Dependent on $\cos\theta=\mathbf{a}\cdot\mathbf{M}$ Rotational invariance

Different events are logically independent:

$$P(x_1,\ldots,x_N|\mathbf{a}\cdot\mathbf{M},Z) \quad = \quad \prod_{i=1}^{N}P(x_i|\theta,Z)$$

The i-prob to observe n_+ and n_- events is

$$P(n_{+1},n_{-1}|\theta,N,Z)=N!\prod_{x=\pm1}\frac{P(x|\theta,Z)^{n_x}}{n_x!}$$

How to express robustness?

- Hypothesis H_0: given θ we observe n_+ and n_-
- Hypothesis H_1: given $\theta+\varepsilon$ we observe n_+ and n_-
- The evidence Ev(H_1/H_0) is given by

$$Ev(H_1 \mid H_0) = \ln \frac{P(n_+, n_- \mid \theta+\varepsilon, N, Z)}{P(n_+, n_- \mid \theta, N, Z)} = \sum_{x=\pm 1} n_x \ln \frac{P(x \mid \theta+\varepsilon, Z)}{P(x \mid \theta, Z)} =$$

$$= \sum_{x=\pm 1} n_x \left\{ \varepsilon \frac{P'(x \mid \theta, Z)}{P(x \mid \theta, Z)} - \frac{\varepsilon^2}{2} \left[\frac{P'(x \mid \theta, Z)}{P(x \mid \theta, Z)} \right]^2 + \frac{\varepsilon^2}{2} \frac{P''(x \mid \theta, Z)}{P(x \mid \theta, Z)} \right\} + O(\varepsilon^3)$$

- Frequencies should be robust with respect to small changes in θ ➔ we should minimize, in absolute value, the coefficients of ε, ε^2,...

Remove dependence on ϵ (1)

$$Ev(H_1 \mid H_0) = \sum_{x=\pm 1} n_x \left\{ \varepsilon \frac{P'(x \mid \theta, Z)}{P(x \mid \theta, Z)} - \frac{\varepsilon^2}{2} \left[\frac{P'(x \mid \theta, Z)}{P(x \mid \theta, Z)} \right]^2 + \frac{\varepsilon^2}{2} \frac{P''(x \mid \theta, Z)}{P(x \mid \theta, Z)} \right\} + O(\varepsilon^3)$$

- Choose $$\boxed{P(x \mid \theta, Z) = \frac{n_x}{N}}$$

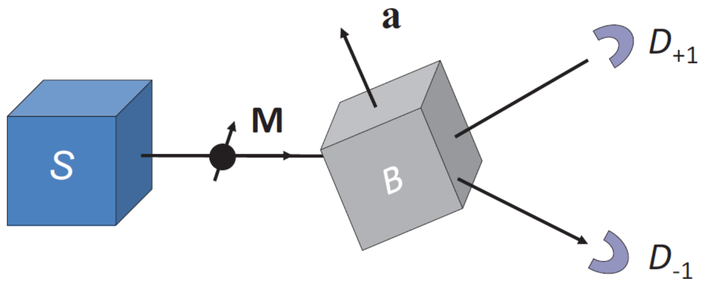
  - Removes the 1st and 3rd term
  - Recover the intuitive procedure of assigning to the i-prob of the individual event, the frequency which maximizes the i-prob to observe the whole data set

Remove dependence on ϵ (2)

$$Ev(H_1 \mid H_0) = \sum_{x=\pm 1} n_x \left\{ \varepsilon \frac{P'(x \mid \theta, Z)}{P(x \mid \theta, Z)} - \frac{\varepsilon^2}{2} \left[\frac{P'(x \mid \theta, Z)}{P(x \mid \theta, Z)} \right]^2 + \frac{\varepsilon^2}{2} \frac{P''(x \mid \theta, Z)}{P(x \mid \theta, Z)} \right\} + O(\varepsilon^3)$$

- Minimizing the 2nd term (Fisher information) for all possible (small) ε and θ

$$\boxed{I_F = \sum_{x=\pm 1} \frac{1}{P(x \mid \theta, Z)} \left(\frac{\partial P(x \mid \theta, Z)}{\partial \theta} \right)^2}$$



$$P(x \mid \mathbf{a} \cdot \mathbf{M}, Z) = P(x \mid \theta, Z) = \frac{1 \pm x \mathbf{a} \cdot \mathbf{M}}{2}$$

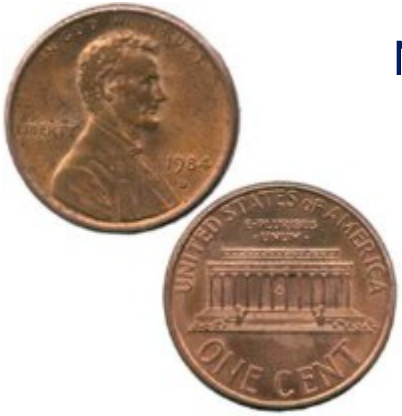
- In agreement with quantum theory of the idealized Stern-Gerlach experiment

Bernoulli trial

Two outcomes (head and tails in coin flypping)

Results are dependent on a single parameter θ which runs a circle (periodicity); what is special in quantum trials?

The results of SG experiment are the most robust, that is, correspond to minimum Fisher information



No assumptions on wave functions, Born rules and other machinery Of quantum physics, just looking for the most robust description of the results of repeating “black box” experiments

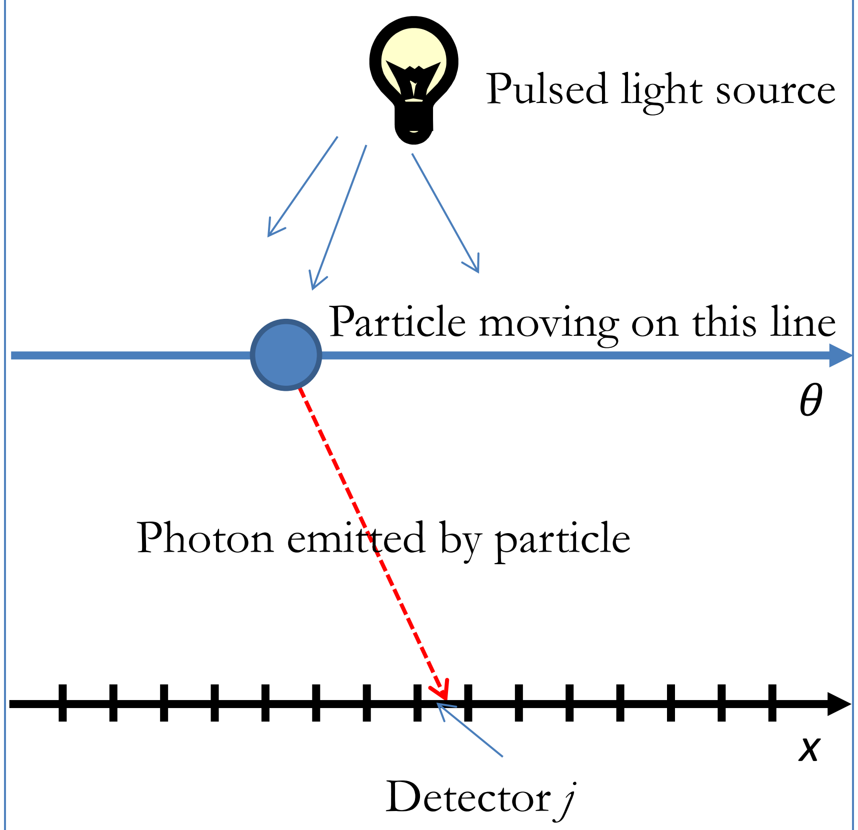
Derivation of basic results of quantum theory by logical inference

- Generic approach
  1. List the features of the experiment that are deemed to be relevant
  2. Introduce the i-prob of individual events
  3. Impose condition of robustness
  4. Minimize functional → equation of quantum theory when applied to experiments in which
     1. There is uncertainty about each event
     2. The conditions are uncertain
     3. Frequencies with which events are observed are reproducible and robust against small changes in the conditions

We need to add some "dynamical" information on the system

Logical inference ➔ Schrödinger equation

- Generic procedure:
- Experiment ➔
- The “true” position θ of the particle is uncertain and remains unknown
- i-prob that the particle at unknown position θ activates the detector at position x : $\boxed{P(x\,|\,\theta,Z)}$



Robustness

- Assume that it does not matter if we repeat the experiment somewhere else ➔

$$\boxed{P(x\,|\,\theta, Z) = P(x+\zeta\,|\,\theta+\zeta, Z) \quad ; \quad \zeta \text{ arbitrary}}$$

- Condition for robust frequency distribution ⬄ minimize the functional (Fisher information)

$$\boxed{I_F(\theta) = \int_{-\infty}^{\infty} dx\, \frac{1}{P(x\,|\,\theta, Z)} \left(\frac{\partial P(x\,|\,\theta, Z)}{\partial x} \right)^2}$$

with respect to $P(x|\theta, Z)$

Impose classical mechanics (á la Schrödinger)

- If there is no uncertainty at all ➔classical mechanics ➔ Hamilton-Jacobi equation

$$\boxed{\frac{1}{2m}\left(\frac{\partial S(\theta)}{\partial \theta}\right)^2 + V(\theta) - E = 0} \qquad \text{(X)}$$

- If there is "known" uncertainty

$$\boxed{\int_{-\infty}^{\infty} dx \left[\left(\frac{\partial S(x)}{\partial x}\right)^2 + 2m[V(x)-E]\right] P(x \mid \theta, Z) = 0} \qquad \text{(XX)}$$

  – Reduces to (X) if $P(x|\theta, Z) \rightarrow \delta(x-\theta)$

Robustness + classical mechanics

- $P(x|\theta, Z)$ can be found by minimizing $I_F(\theta)$ with the constraint that (XX) should hold

➔ We should minimize the functional

$$\boxed{F(\theta) = \int_{-\infty}^{\infty} dx \left\{ \frac{1}{P(x\,|\,\theta, Z)} \left(\frac{\partial P(x\,|\,\theta, Z)}{\partial x} \right)^2 + \lambda \left[\left(\frac{\partial S(x)}{\partial x} \right)^2 + 2m[V(x) - E] \right] P(x\,|\,\theta, Z) \right\}}$$

  - λ = Lagrange multiplier
  - Nonlinear equations for $P(x|\theta, Z)$ and $S(x)$

Robustness + classical mechanics

- Nonlinear equations for $P(x|\theta, Z)$ and $S(x)$ can be turned into linear equations by substituting*

$$\boxed{\psi(x\mid\theta,Z)=\sqrt{P(x\mid\theta,Z)}e^{iS(x)\sqrt{\lambda}/2}} \quad \rightarrow$$

$$\boxed{F(\theta)=\int_{-\infty}^{\infty}dx\left\{4\frac{\partial\psi^*(x\mid\theta,Z)}{\partial x}\frac{\partial\psi(x\mid\theta,Z)}{\partial x}+2m\lambda[V(x)-E]\psi^*(x\mid\theta,Z)\psi(x\mid\theta,Z)\right\}}$$

- Minimizing with respect to $\psi(x\mid\theta,Z)$ yields

$$\boxed{-\frac{\partial^2\psi(x\mid\theta,Z)}{\partial x^2}+\frac{m\lambda}{2}\left[V(x)-E\right]\psi(x\mid\theta,Z)=0}$$

$\rightarrow$ Schrödinger equation $\lambda = 4K^{-2} = 4\hbar^{-2}$

*E. Madelung, "Quantentheorie in hydrodynamischer Form," Z. Phys. 40, 322 – 326 (1927)

Time-dependent, multidimensional case

The space is filled by detectors which are fired (or not fired) at some discrete (integer) time $\tau = 1, \ldots, M$

At the very end we have a set of data presented as 0 (no particle in a given box at a given instant or 1

$$\Upsilon = \{\boldsymbol{j}_{n,\tau} | \boldsymbol{j}_{n,\tau} \in [-L^d, L^d];\ n = 1, \ldots, N;\ \tau = 1, \ldots, M\}$$

or, denoting the total counts of voxels $\boldsymbol{j}$ at time τ by $0 \leq k_{\boldsymbol{j},\tau} \leq N$, the experiment produces the data set

$$\mathcal{D} = \left\{ k_{\boldsymbol{j},\tau} \middle| \tau = 1, \ldots, M; N = \sum_{\boldsymbol{j} \in [-L^d, L^d]} k_{\boldsymbol{j},\tau} \right\}. \tag{55}$$

Logical independence of events:

$$P(\mathcal{D}|\theta_1, \ldots, \theta_M, N, Z) = N! \prod_{\tau=1}^{M} \prod_{\boldsymbol{j} \in [-L^d, L^d]} \frac{P(\boldsymbol{j}|\theta_\tau, \tau, Z)^{k_{\boldsymbol{j},\tau}}}{k_{\boldsymbol{j},\tau}!}$$

Time-dependent case II

Homogeneity of the space: $P(\boldsymbol{j}|\boldsymbol{\theta}, Z) = P(\boldsymbol{j}+\boldsymbol{\zeta}|\boldsymbol{\theta}+\boldsymbol{\zeta}, Z)$

Evidence: $$\mathrm{Ev} = \sum_{\boldsymbol{j},\tau} \sum_{i,i'=1}^{d} \frac{\epsilon_{i,\tau}\epsilon_{i',\tau}}{P(\boldsymbol{j}|\boldsymbol{\theta}_\tau, \tau, Z)} \frac{\partial P(\boldsymbol{j}|\boldsymbol{\theta}_\tau, \tau, Z)}{\partial \theta_i} \frac{\partial P(\boldsymbol{j}|\boldsymbol{\theta}_\tau, \tau, Z)}{\partial \theta_{i'}}$$

$$\mathrm{Ev} = \sum_{\boldsymbol{j},\tau} \left(\sum_{i=1}^{d} \frac{\epsilon_i,\, \tau}{\sqrt{P(\boldsymbol{j}|\boldsymbol{\theta}_\tau, \tau, Z)}} \frac{\partial P(\boldsymbol{j}|\boldsymbol{\theta}_\tau, \tau, Z)}{\partial \theta_i} \right)^2 \geq 0,$$

and, by using the Cauchy–Schwarz inequality, that

$$\mathrm{Ev} \leq \sum_{\boldsymbol{j},\tau} \left(\sum_{i=1}^{d} \epsilon_{i,\tau}^2 \right) \left(\sum_{i=1}^{d} \frac{1}{P(\boldsymbol{j}|\boldsymbol{\theta}_\tau, \tau, Z)} \left(\frac{\partial P(\boldsymbol{j}|\boldsymbol{\theta}_\tau, \tau, Z)}{\partial \theta_i} \right)^2 \right)$$

$$\widehat{\epsilon}^2 = \max_{i,\tau} \epsilon_{i,\tau}^2$$

$$\leq d\widehat{\epsilon}^2 \sum_{\boldsymbol{j},\tau} \sum_{i=1}^{d} \frac{1}{P(\boldsymbol{j}|\boldsymbol{\theta}_\tau, \tau, Z)} \left(\frac{\partial P(\boldsymbol{j}|\boldsymbol{\theta}_\tau, \tau, Z)}{\partial \theta_i} \right)^2,$$

Time-dependent case III

Minimizing Fisher information: $$I_F = \sum_{\boldsymbol{j},\tau} \sum_{i=1}^{d} \frac{1}{P(\boldsymbol{j}|\boldsymbol{\theta}_\tau, \tau, Z)} \left(\frac{\partial P(\boldsymbol{j}|\boldsymbol{\theta}_\tau, \tau, Z)}{\partial \theta_i} \right)^2$$

Taking into account homogeneity of space; continuum limit:

$$I_F = \int d\boldsymbol{x} \int dt \sum_{i=1}^{d} \frac{1}{P(\boldsymbol{x}|\boldsymbol{\theta}(t), t, Z)} \left(\frac{\partial P(\boldsymbol{x}|\boldsymbol{\theta}(t), t, Z)}{\partial x_i} \right)^2$$

Hamilton – Jacobi equations:

$$\frac{\partial S(\boldsymbol{\theta}, t)}{\partial t} + \frac{1}{2m} \left(\nabla S(\boldsymbol{\theta}, t) - \frac{q}{c} \mathbf{A}(\boldsymbol{\theta}, t) \right)^2 + V(\boldsymbol{\theta}, t) = 0$$

Time-dependent case IV

Minimizing functional:

$$F = \int d\boldsymbol{x} \int dt \sum_{i=1}^{d} \left\{ \frac{1}{P(\boldsymbol{x}|\boldsymbol{\theta}(t),t,Z)} \left(\frac{\partial P(\boldsymbol{x}|\boldsymbol{\theta}(t),t,Z)}{\partial x_i} \right)^2 + \lambda \left[\frac{\partial S(\boldsymbol{x},t)}{\partial t} + \frac{1}{2m} \left(\frac{\partial S(\boldsymbol{x},t)}{\partial x_i} - \frac{q}{c}\mathbf{A}(\boldsymbol{x},t) \right)^2 + V(\boldsymbol{x},t) \right] P(\boldsymbol{x}|\boldsymbol{\theta}(t),t,Z) \right\}$$

Substitution $\psi(\boldsymbol{x}|\boldsymbol{\theta}(t),t,Z) = \sqrt{P(\boldsymbol{x}|\boldsymbol{\theta}(t),t,Z)}\, e^{iS(\boldsymbol{x},t)\sqrt{\lambda}/2}$

Equivalent functional for minimization:

$$\begin{aligned} Q = 2 \int d\boldsymbol{x} \int dt \, \Bigg\{ & mi\sqrt{\lambda} \left[\psi(\boldsymbol{x}|\boldsymbol{\theta}(t),t,Z) \frac{\partial \psi^*(\boldsymbol{x}|\boldsymbol{\theta}(t),t,Z)}{\partial t} - \psi^*(\boldsymbol{x}|\boldsymbol{\theta}(t),t,Z) \frac{\partial \psi(\boldsymbol{x}|\boldsymbol{\theta}(t),t,Z)}{\partial t} \right] \\ & + 2 \sum_{j=1}^{d} \left(\frac{\partial \psi^*(\boldsymbol{x}|\boldsymbol{\theta}(t),t,Z)}{\partial x_j} + \frac{iq\sqrt{\lambda}}{2c} A_j(\boldsymbol{x},t) \psi^*(\boldsymbol{x}|\boldsymbol{\theta}(t),t,Z) \right) \\ & \times \left(\frac{\partial \psi(\boldsymbol{x}|\boldsymbol{\theta}(t),t,Z)}{\partial x_j} - \frac{iq\sqrt{\lambda}}{2c} A_j(\boldsymbol{x},t) \psi(\boldsymbol{x}|\boldsymbol{\theta}(t),t,Z) \right) \\ & + m\lambda V(\boldsymbol{x},t) \psi^*(\boldsymbol{x}|\boldsymbol{\theta}(t),t,Z) \psi(\boldsymbol{x}|\boldsymbol{\theta}(t),t,Z) \Bigg\}, \end{aligned}$$

$$\lambda = 4/\hbar^2$$

Time-dependent case V

Time-dependent Schrödinger equation

$$i\hbar \frac{\partial \psi(\boldsymbol{x}|\boldsymbol{\theta}(t), t, Z)}{\partial t} = \left[-\frac{\hbar^2}{2m} \sum_{j=1}^{d} \left(\frac{\partial}{\partial x_j} - \frac{iq}{\hbar c} \boldsymbol{A}(\boldsymbol{x}, t) \right)^2 + V(x, t) \right] \psi(\boldsymbol{x}|\boldsymbol{\theta}(t), t, Z)$$

It is linear (superposition principle) which follows from classical Hamiltonian (kinetic energy is $mv^2/2$) and, inportantly, from building one complex function from two real (S and S +2πħ are equivalent).

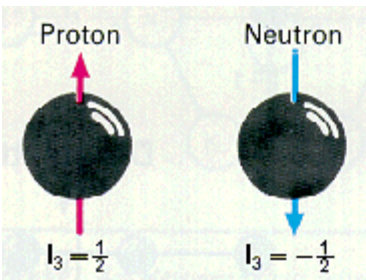
A very nontrivial operation dictated just by desire to simplify the problem as much as possible (to pass from nonlinear to linear equation).

Requires further careful thinking!

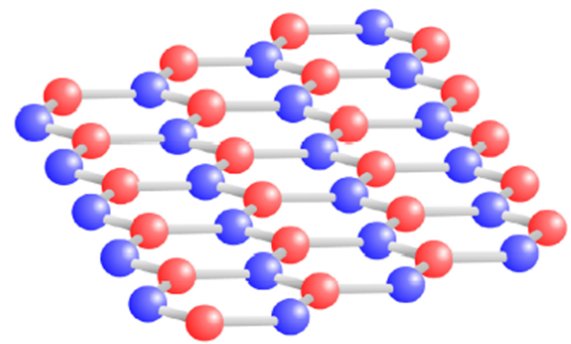
Pauli equation

What is spin? Just duality (e.g., color – blue or red). Nothing is rotating (yet!)

Isospin in nuclear physics



Sublattice index in graphene



Just add color (*k*=1,2)

The result of N repetitions of the experiment yields the data set

$$\Upsilon = \{(\mathbf{j}, k)_{n,\tau} | \mathbf{j}_{n,\tau} \in \mathcal{V};\ k = \pm 1;\ n = 1, \dots, N;\ \tau = 1, \dots, M\}, \tag{1}$$

or, denoting the total counts of voxels $\mathbf{j}$ and color k at time τ by $0 \le c_{\mathbf{j},k,\tau} \le N$, the data set can be represented as

$$\mathcal{D} = \left\{ c_{\mathbf{j},k,\tau} \middle| \tau = 1, \dots, M\ ;\ \sum_{k=\pm 1} \sum_{\mathbf{j} \in [-L^d, L^d]} c_{\mathbf{j},k,\tau} = N \right\}. \tag{2}$$

Pauli equation II

Fisher information part just copies the previous derivation

$$\mathrm{Ev} = \ln \frac{P(\mathcal{D}|\mathbf{X}_\tau + \boldsymbol{\varepsilon}_\tau, \tau, N, Z)}{P(\mathcal{D}|\mathbf{X}_\tau, \tau, N, Z)}$$

$$= \sum_{\mathbf{j},k,\tau} c_{\mathbf{j},k,\tau} \ln \frac{P(\mathbf{j}, k|\mathbf{X}_\tau + \boldsymbol{\varepsilon}_\tau, \tau, Z)}{P(\mathbf{j}, k|\mathbf{X}_\tau, \tau, Z)}$$

for the evidence

Expansion

$$\mathrm{Ev} = \sum_{\mathbf{j},k,\tau} c_{\mathbf{j},k,\tau} \ln \left[1 + \frac{\boldsymbol{\varepsilon}_\tau \cdot \boldsymbol{\nabla}_\tau P(\mathbf{j}, k|\mathbf{X}_\tau, \tau, Z)}{P(\mathbf{j}, k|\mathbf{X}_\tau, \tau, Z)} + \frac{1}{2} \frac{(\boldsymbol{\varepsilon}_\tau \cdot \boldsymbol{\nabla}_\tau)^2 P(\mathbf{j}, k|\mathbf{X}_\tau, \tau, Z)}{P(\mathbf{j}, k|\mathbf{X}_\tau, \tau, Z)} + \mathcal{O}(\varepsilon_\tau^3) \right]$$

$$= \sum_{\mathbf{j},k,\tau} c_{\mathbf{j},k,\tau} \left[\frac{\boldsymbol{\varepsilon}_\tau \cdot \boldsymbol{\nabla}_\tau P(\mathbf{j}, k|\mathbf{X}_\tau, \tau, Z)}{P(\mathbf{j}, k|\mathbf{X}_\tau, \tau, Z)} - \frac{1}{2} \left[\frac{\boldsymbol{\varepsilon}_\tau \cdot \boldsymbol{\nabla}_\tau P(\mathbf{j}, k|\mathbf{X}_\tau, \tau, Z)}{P(\mathbf{j}, k|\mathbf{X}_\tau, \tau, Z)} \right]^2 \right.$$

$$\left. + \ \frac{1}{2} \frac{(\boldsymbol{\varepsilon}_\tau \cdot \boldsymbol{\nabla}_\tau)^2 P(\mathbf{j}, k|\mathbf{X}_\tau, \tau, Z)}{P(\mathbf{j}, k|\mathbf{X}_\tau, \tau, Z)} \right] + \mathcal{O}(\boldsymbol{\varepsilon}_\tau^3),$$

Pauli equation III

$$I_F = \sum_{\mathbf{j},k,\tau} \frac{1}{P(\mathbf{j},k|\mathbf{X}_\tau,\tau,Z)} \left[\nabla_\tau P(\mathbf{j},k|\mathbf{X}_\tau,\tau,Z)\right]^2 = \int d\mathbf{x}\,dt \sum_{k=\pm 1} \frac{1}{P(\mathbf{x},k|\mathbf{X},t,Z)} \left[\nabla P(\mathbf{x},k|\mathbf{X},t,Z)\right]^2$$

$$P(\mathbf{x},k=+1|\mathbf{X},t,Z) = P(\mathbf{x}|\mathbf{X},t,Z)\cos^2\frac{\theta(\mathbf{x},\mathbf{X},t,Z)}{2}$$

$$P(\mathbf{x},k=-1|\mathbf{X},t,Z) = P(\mathbf{x}|\mathbf{X},t,Z)\sin^2\frac{\theta(\mathbf{x},\mathbf{X},t,Z)}{2}$$

$$I_F = \int d\mathbf{x}\,dt \left\{ \frac{1}{P(\mathbf{x}|\mathbf{X},t,Z)} \left[\nabla P(\mathbf{x}|\mathbf{X},t,Z)\right]^2 + \left[\nabla\theta(\mathbf{x},\mathbf{X},t,Z)\right]^2 P(\mathbf{x}|\mathbf{X},t,Z) \right\}$$

$\theta(\mathbf{x},\mathbf{X},t,Z)$ has no dynamical or geometric meaning (yet)

Pauli equation IV

Dynamical part is less trivial; we restrict ourselves only by d=3 (spin is introduced in 3D space, it is important!)

Alternative representation of the Newton's laws (or HJE)

$$\frac{d\mathbf{x}}{dt} = \mathbf{U}(\mathbf{x}, t)$$ The velocity field is derived by (numerical) differentiation of position data

Decomposition for any vector field in 3D:

$$\mathbf{U}(\mathbf{x}, t) = \nabla S(\mathbf{x}, t) - \mathbf{A}(\mathbf{x}, t)$$

$$\mathbf{A}(\mathbf{x}, t) = \nabla \times \mathbf{W}(\mathbf{x}, t)$$

$$\nabla \cdot \mathbf{A} = 0$$

Direct differentiation:

$$\begin{aligned}
\frac{d^2 x_i}{dt^2} &= \frac{\partial U_i}{\partial t} + \sum_{j=1}^{3} \frac{\partial U_i}{\partial x_j} U_j \\
&= \frac{\partial^2 S}{\partial x_i \partial t} - \frac{\partial A_i}{\partial t} + \sum_{j=1}^{3} \left(\frac{\partial^2 S}{\partial x_i \partial x_j} - \frac{\partial A_i}{\partial x_j} \right) \left(\frac{\partial S}{\partial x_j} - A_j \right) \\
&= \frac{\partial}{\partial x_i} \left[\frac{\partial S}{\partial t} + \frac{1}{2} \sum_{j=1}^{3} \left(\frac{\partial S}{\partial x_j} - A_j \right)^2 \right] + \sum_{j=1}^{3} \left(\frac{\partial A_j}{\partial x_i} - \frac{\partial A_i}{\partial x_j} \right) \left(\frac{\partial S}{\partial x_j} - A_j \right) - \frac{\partial A_i}{\partial t}
\end{aligned}$$

Pauli equation V

Introducing the vector field $\mathbf{B} = \nabla \times \mathbf{A}$

$$\frac{d^2\mathbf{x}}{dt^2} = \nabla\left[\frac{\partial S}{\partial t} + \frac{1}{2}(\nabla S - \mathbf{A})^2\right] + \frac{d\mathbf{x}}{dt} \times \mathbf{B} - \frac{\partial \mathbf{A}}{\partial t}$$

Hypothesis (alternative form of HJE): Existence of scalar field $\phi(\mathbf{x}, t)$

such that $$\frac{\partial S}{\partial t} + \frac{1}{2}(\nabla S - \mathbf{A})^2 = -\phi$$

Then, upon introducing the vector field $\mathbf{E} = -\nabla\phi - \partial\mathbf{A}/\partial t$,

$$\frac{d^2\mathbf{x}}{dt^2} = \mathbf{E} + \frac{d\mathbf{x}}{dt} \times \mathbf{B}.$$

Nothing but equation of motion of particle in electromagnetic field (in proper units)

Pauli equation VI

Dynamical information on the system (constrain):

we will require that there exists two scalar fields $V_k(\mathbf{x},t)$ for $k=\pm1$ such that

$$\int d\mathbf{x}\,dt \sum_{k=\pm1}\left[\frac{\partial S_k(\mathbf{x},t)}{\partial t}+\frac{1}{2m}\left(\nabla S_k(\mathbf{x},t)-q\mathbf{A}(\mathbf{x},t)\right)^2+V_k(\mathbf{x},t)\right]P(\mathbf{x},k|\mathbf{X},t,Z)=0,$$

$$S_k(\mathbf{x},t)=S(\mathbf{x},t)-kR(\mathbf{x},t) \text{ for } k=\pm1$$

$$V_0(\mathbf{x},t)=[V_{+1}(\mathbf{x},t)+V_{-1}(\mathbf{x},t)]/2,\ V_1(\mathbf{x},t)=[V_{+1}(\mathbf{x},t)-V_{-1}(\mathbf{x},t)]/2$$

Constrain functional:

$$\begin{aligned}
\Lambda &= \int d\mathbf{x}\,dt \sum_{k=\pm1}\left[\frac{\partial S_k(\mathbf{x},t)}{\partial t}+\frac{1}{2m}\left(\nabla S_k(\mathbf{x},t)-q\mathbf{A}(\mathbf{x},t)\right)^2+V_k(\mathbf{x},t)\right]P(\mathbf{x},k|\mathbf{X},t,Z)\\
&= \int d\mathbf{x}\,dt\left\{\frac{1}{2m}\left[(\nabla S(\mathbf{x},t)-q\mathbf{A}(\mathbf{x},t))^2+\left(\nabla R(\mathbf{x},t)\right)^2\right.\right.\\
&\quad \left.-\,2\cos\theta(\mathbf{x},\mathbf{X},t,Z)\nabla R(\mathbf{x},t)\left(\nabla S(\mathbf{x},t)-q\mathbf{A}(\mathbf{x},t)\right)\right]\\
&\quad +\left[\frac{\partial S(\mathbf{x},t)}{\partial t}-\cos\theta(\mathbf{x},\mathbf{X},t,Z)\frac{\partial R(\mathbf{x},t)}{\partial t}\right]+V_0(\mathbf{x},t)\\
&\quad \left.+\,V_1(\mathbf{x},t)\cos\theta(\mathbf{x},\mathbf{X},t,Z)\right\}P(\mathbf{x}|\mathbf{X},t,Z),
\end{aligned}$$

Pauli equation VII

Up to know we did not assume that "color" is related to any rotation or any magnetic moment. But we know experimentally (anomalous Zeeman effect) that electron has magnetic moment, with its energy in external magnetic field $\widehat{V}_1(\mathbf{x},t) = -\gamma\,\mathbf{m}(\mathbf{x},t)\cdot\mathbf{B}(\mathbf{x},t)$. We have correct classical equations of precession if we identify $\theta(\mathbf{x},\mathbf{X},t,Z)$ and $\varphi(\mathbf{x},t) = R(\mathbf{x},t)/a$ with the polar angles of the unit vector $\mathbf{m}(\mathbf{x},t)$

$$
\begin{aligned}
\Lambda = \int d\mathbf{x}\,dt \Bigg\{ & \frac{1}{2m}\Big[(\nabla S(\mathbf{x},t) - q\mathbf{A}(\mathbf{x},t))^2 + a^2\big(\nabla\varphi(\mathbf{x},t)\big)^2 \\
& - 2a\cos\theta(\mathbf{x},\mathbf{X},t,Z)\nabla\varphi(\mathbf{x},t)\,(\nabla S(\mathbf{x},t) - q\mathbf{A}(\mathbf{x},t))\Big] \\
& + \left[\frac{\partial S(\mathbf{x},t)}{\partial t} - a\cos\theta(\mathbf{x},\mathbf{X},t,Z)\frac{\partial\varphi(\mathbf{x},t)}{\partial t}\right] + V_0(\mathbf{x},t) \\
& - a\gamma\,\mathbf{m}(\mathbf{x},t)\cdot\mathbf{B}(\mathbf{x},t)\Bigg\} P(\mathbf{x}|\mathbf{X},t,Z).
\end{aligned}
$$

Pauli equation VIII

$$V_0(\mathbf{x}, t) = q\phi(\mathbf{x}, t), a = \hbar/2, \gamma = q/m \quad \lambda = \hbar^2/8m$$

$$\Phi(\mathbf{x}, t) = \begin{pmatrix} P^{1/2}(\mathbf{x}, k = +1|\mathbf{X}, t, Z)e^{iS_1(\mathbf{x},t)/\hbar} \\ P^{1/2}(\mathbf{x}, k = -1|\mathbf{X}, t, Z)e^{iS_2(\mathbf{x},t)/\hbar} \end{pmatrix}$$

Extremum of the functional $F = \lambda I_F + \Lambda$

gives the Pauli equation: $i\hbar \frac{\partial}{\partial t}\Phi = H\Phi$

$$\begin{aligned} H &= \frac{1}{2m}\{\boldsymbol{\sigma} \cdot [-i\hbar\nabla - q\mathbf{A}(\mathbf{x}, t)]\}^2 + q\phi(\mathbf{x}, t) \\ &= \frac{1}{2m}[-i\hbar\nabla - q\mathbf{A}(\mathbf{x}, t)]^2 + q\phi(\mathbf{x}, t) - \frac{q\hbar}{2m}\boldsymbol{\sigma} \cdot \mathbf{B}(\mathbf{x}, t) \end{aligned}$$

$$\boldsymbol{\sigma} = (\sigma^x, \sigma^y, \sigma^z)^T$$

Separation of conditions principle

Separation of conditions as a prerequisite for quantum theory

Annals of Physics 403 (2019) 112–135

Hans De Raedt [a], Mikhail I. Katsnelson [b], Dennis Willsch [c], Kristel Michielsen [c,d,*]

LI allows to derive also Pauli equation, Klein-Gordon equation (Dirac is in progress) but... Superposition principle arises as a trick. Why linear equation? Why wave function? Last not least – what about *open* quantum systtems?

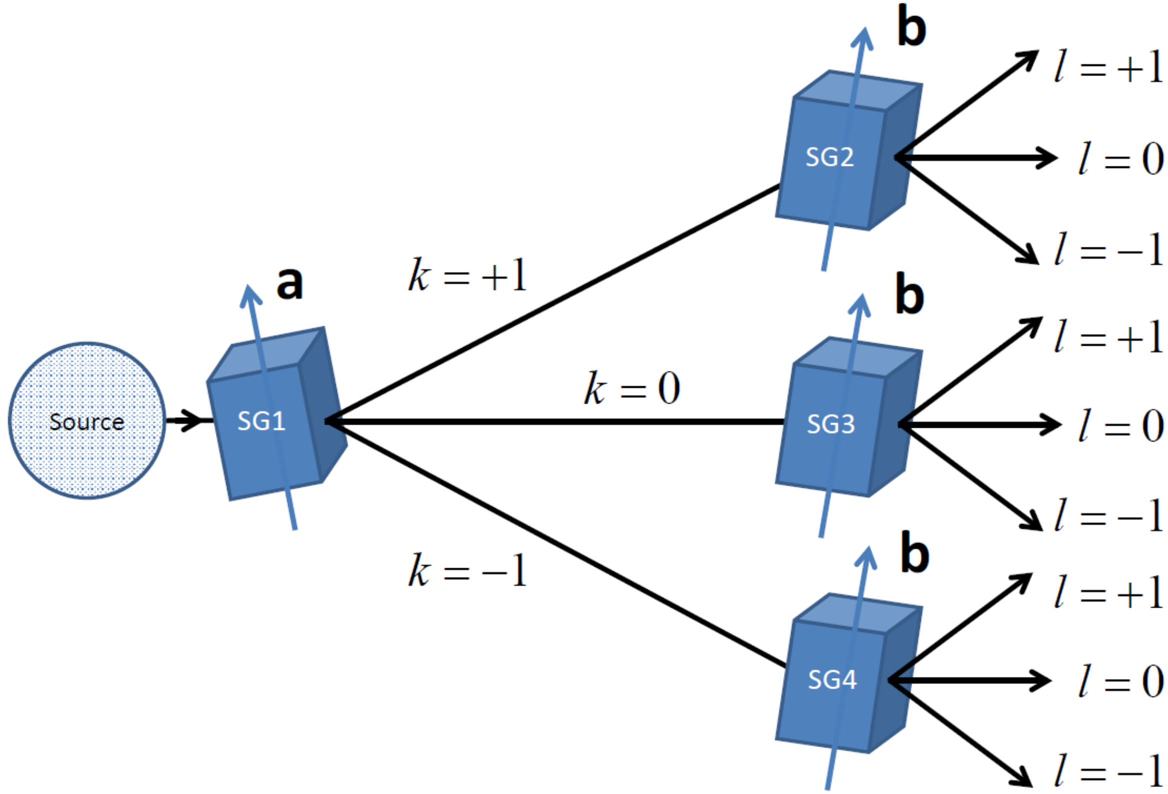
Slightly different view but also based on data analysis

Standard logic: Shrödinger equation ⟶ von Neumann prescription ⟶ description of meaurements. We invert this logic!

Starting point: the way how we deal with the data (reproduced as binary sequences)

Separation procedure

Double SG experiment with three possible outcomes ("spin 1") is generic enough



The first SG device prepares the initial state for the second device

Separation procedure II

The data set for the first device

$$\mathscr{K} = \{k_n \mid k_n \in \{+1, 0, -1\}\ ;\ n = 1, \ldots, N\}$$

$$f(k|\mathbf{a}, P, N) = \frac{1}{N} \sum_{n=1}^{N} \delta_{k,k_n}$$

P properties of the particles emitted by source

Representation in terms of momenta

$$f(k|\mathbf{a}, P, N) = 1 - m_2(\mathbf{a}, P, N) + \frac{m_1(\mathbf{a}, P, N)}{2} k + \frac{3m_2(\mathbf{a}, P, N) - 2}{2} k^2$$

$$m_p(\mathbf{a}, P, N) = \langle k^p \rangle_{\mathbf{a}} = \frac{1}{N} \sum_{n=1}^{N} k_n^p = \sum_{k=+1,0,-1} k^p f(k|\mathbf{a}, P, N) \quad , \quad p = 0, 1, 2$$

Separation procedure III

Let us try to represent the data as strings (sequences)

$$\mathbf{k} = (+1, 0, -1)^T \qquad \mathbf{f} = (f(+1|\mathbf{a}, P, N), f(0|\mathbf{a}, P, N), f(-1|\mathbf{a}, P, N))^T$$

$$\langle 1 \rangle_{\mathbf{a}} = (1,1,1) \cdot \mathbf{f} = \mathbf{Tr}\,(1,1,1) \cdot \mathbf{f} = \mathbf{Tr}\,\mathbf{f} \cdot (1,1,1) = \mathbf{Tr} \begin{pmatrix} f(+1|\mathbf{a}, P, N) & 0 & 0 \\ 0 & f(0|\mathbf{a}, P, N) & 0 \\ 0 & 0 & f(-1|\mathbf{a}, P, N) \end{pmatrix}$$

$$\langle k \rangle_{\mathbf{a}} = \mathbf{k}^T \cdot \mathbf{f} = \mathbf{Tr}\,\mathbf{k}^T \cdot \mathbf{f} = \mathbf{Tr}\,\mathbf{f} \cdot \mathbf{k}^T = \mathbf{Tr} \begin{pmatrix} f(+1|\mathbf{a}, P, N) & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -f(-1|\mathbf{a}, P, N) \end{pmatrix}$$

$\langle k^2 \rangle_{\mathbf{a}} = \mathbf{Tr}\,\mathbf{f} \cdot (\mathbf{k}^{(2)})^T \qquad \mathbf{k}^{(2)} = (+1, 0, +1)^T$ is the other vector

Separation procedure IV

But with matrice multiplication rule we need only two matrices

$$\widetilde{\mathbf{K}} = \begin{pmatrix} +1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix} \quad \text{and} \quad \widetilde{\mathbf{F}}(\mathbf{a},P,N) = \begin{pmatrix} f(+1|\mathbf{a},P,N) & 0 & 0 \\ 0 & f(0|\mathbf{a},P,N) & 0 \\ 0 & 0 & f(-1|\mathbf{a},P,N) \end{pmatrix}$$

$$\langle k^p \rangle_{\mathbf{a}} = \mathbf{Tr}\,\widetilde{\mathbf{F}}(\mathbf{a},P,N)\widetilde{\mathbf{K}}^p \quad , \quad p = 0,1,2$$

When we rotate the axis of the first SG device and assume rotational invariance (+1 means along the device axis, -1 means opposite, 0 means perpendicular to the axis, for any direction of the axis)

$$\mathbf{K}(\mathbf{a}) = \mathbf{a} \cdot \mathbf{S} \qquad S^x = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \quad , \quad S^y = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & -i & 0 \\ +i & 0 & -i \\ 0 & +i & 0 \end{pmatrix} \quad , \quad S^z = \begin{pmatrix} +1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

Nothing is quantum yet, except the assumption of *three* outcomes!

Separation procedure V

$$\mathbf{M}_k(\mathbf{e}_z) = \mathbb{1} - (S^z)^2 + \frac{k}{2}S^z + \frac{k^2}{2}\left[3(S^z)^2 - 2\mathbb{1}\right]$$

Introduce projector operator:

$$\mathbf{M}_k(\mathbf{e}_z)\mathbf{M}_l(\mathbf{e}_z) = \delta_{k,l}\mathbf{M}_k(\mathbf{e}_z)$$

$$= \begin{pmatrix} \frac{k^2+k}{2} & 0 & 0 \\ 0 & 1-k^2 & 0 \\ 0 & 0 & \frac{k^2-k}{2} \end{pmatrix} = \begin{cases} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, & k=+1 \\ \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix}, & k=0 \\ \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}, & k=-1 \end{cases}$$

From rotational invariance:

$$\mathbf{M}_k(\mathbf{a}) = 1 - (\mathbf{a}\cdot\mathbf{S})^2 + \frac{k}{2}\mathbf{a}\cdot\mathbf{S} + \frac{k^2}{2}\left[3(\mathbf{a}\cdot\mathbf{S})^2 - 2\mathbb{1}\right]$$

$$f(k|\mathbf{a},P,N) = \mathbf{Tr}\,\mathbf{F}(P,N)\mathbf{M}_k(\mathbf{a}) = \mathbf{Tr}\,\mathbf{M}_k(\mathbf{a})\mathbf{F}(P,N) = \mathbf{Tr}\,\mathbf{M}_k(\mathbf{a})\mathbf{F}(P,N)\mathbf{M}_k(\mathbf{a})$$

Only the last form gives Hermitian density matrix for the next use!

Separation procedure VI

As all SG magnets are assumed to be identical, consistency demands that their description should be the same, that is the filtering property of SG2, SG3 and SG4 should be described by $\mathbf{M}_l(\mathbf{b})$.

The first SG device plays the role of the source for the second device etc. – this is the separaction of conditions requirement!

$$\mathscr{D} = \left\{ (k_n, l_n) \mid k_n, l_n \in \{+1, 0, -1\} \, ; \, n = 1, \ldots, N \right\}$$

$$f(k|\mathbf{a}, P, N) = \sum_{l=+1,0,-1} f(k, l|\mathbf{a}, \mathbf{b}, P, N)$$

$$f(k, l|\mathbf{a}, \mathbf{b}, P, N) = \mathbf{Tr}\, \mathbf{M}_l(\mathbf{b}) \mathbf{M}_k(\mathbf{a}) \mathbf{F}(P, N) \mathbf{M}_k(\mathbf{a}) \mathbf{M}_l(\mathbf{b})$$

Consequence: $$f(k|\mathbf{a}, P, N) = \sum_{l=+1,0,-1} f(k, l|\mathbf{a}, \mathbf{b}, P, N)$$

Separation procedure VII

Until now *P* (the properties of source) is arbitrary. Illustration:

$$\mathbf{F}(P,N) = \frac{1}{3}\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \qquad f(k|\mathbf{a},P,N) = \mathbf{Tr}\,\mathbf{M}_k(\mathbf{a})\mathbf{F}(P,N)\mathbf{M}_k(\mathbf{a}) = \frac{1}{3}$$

(sourse of unpolarized particles, full isotropy in single SG)

$$\begin{aligned} f(k,l|\mathbf{a},\mathbf{b},P,N) &= \mathbf{Tr}\,\mathbf{M}_l(\mathbf{b})\mathbf{M}_k(\mathbf{a})\mathbf{F}(P,N)\mathbf{M}_k(\mathbf{a})\mathbf{M}_l(\mathbf{b}) \\ &= \begin{cases} \frac{1}{12}(1+\mathbf{a}\cdot\mathbf{b})^2 \quad , \quad k=l=+1,-1 \\ \frac{1}{3}(\mathbf{a}\cdot\mathbf{b})^2 \quad , \quad k=l=0 \\ \frac{1}{12}(1-\mathbf{a}\cdot\mathbf{b})^2 \quad , \quad (k,l)=(+1,-1),(-1,+1) \\ \frac{1}{6}(1-(\mathbf{a}\cdot\mathbf{b})^2) \quad , \quad (k,l)=(+1,0),(-1,0),(0,+1),(0,-1) \end{cases} \end{aligned}$$

This is the result of QM – but strictly speaking not the *derivation*

$$\mathrm{SOC} \models \mathrm{QT}$$

Separation procedure VIII

Dependence on parameters (e.g., time) $\mathscr{D}(\lambda)$ $f(k,l|\mathbf{a},\mathbf{b},P,N,\lambda)$

$$\langle k^p\rangle_\lambda = \mathbf{Tr}\,\mathbf{F}(P,N,\lambda)\mathbf{K}^p(\mathbf{a}) \quad , \quad p=0,1,2$$

$$\mathbf{Tr}\,\mathbf{F}(P,N,\lambda)=1 \qquad \mathbf{Tr}\,\frac{\partial^n\mathbf{F}(P,N,\lambda)}{\partial\lambda^n}=0 \quad , \quad n>0$$

Traceless matrix is a commutator

K. Shoda, “Einige Sätze über Matrizen,” Jap. J. Math. **13**, 361–365 (1936).
A. A. Albert and B. Muckenhoupt, “On matrices of trace zeros,” Michigan Math. J. , 1–3 (1957).

$$\frac{\partial\mathbf{F}(P,N,\lambda)}{\partial\lambda}=[Y(\lambda),Z(\lambda)]$$

$\mathbf{F}(P,N,\lambda)$ is a Hermitian (non-negative definite) matrix

$\mathbf{F}(P,N,\lambda)=U^\dagger(\lambda)D(\lambda)U(\lambda)$ $D(\lambda)$ is diagonal

Separation procedure IX

$$\frac{\partial \mathbf{F}(P,N,\lambda)}{\partial \lambda} = \left[\mathbf{F}(P,N,\lambda), U^{\dagger}(\lambda)\frac{\partial U(\lambda)}{\partial \lambda}\right] + U^{\dagger}(\lambda)\frac{\partial D(\lambda)}{\partial \lambda}U(\lambda)$$

If we assume $\partial D(\lambda)/\partial \lambda = 0$ $\quad \frac{\partial \mathbf{F}(P,N,\lambda)}{\partial \lambda} = i[\mathbf{F}(P,N,\lambda), H(\lambda)]$

$iH(\lambda) = U^{\dagger}(\lambda)(\partial U(\lambda)/\partial \lambda)$

H is Hermitian and cannot dependent on *F* due to separation requirement

Von Neumann equation:

$$i\hbar\frac{\partial \rho(t)}{\partial t} = [H(t), \rho(t)]$$

If $\rho(t) = |\Psi(t)\rangle\langle\Psi(t)|$ (its eigenvalues are not dependent on time in this case!)

we have Schrödinger equation $i\hbar\frac{\partial}{\partial t}|\Psi(t)\rangle = H(t)|\Psi(t)\rangle$

but to find the “Hamiltonian” one needs other considerations (e.g. like in logical inference part)

To conclude

The way how we deal organize the “data” adds a lot of restrictions on mathematical apparatus which deals with predictions of outcomes of *uncertain* measurements (QT does not predict individual outcomes): (1) Robustness and (2) Separation of conditions

It is not enough to derive QM as a unique theory, some physics should be added but in restricts enormously a class of possible theories

Even if God does not play dice we have to describe the world as if He does

A lot of thing to do but, at least, one can replace (some) (quasi)philosophical declarations by calculations – as we like

Thank you