Radboud Universiteit







# **Does God play dice?**

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# References

# Quantum theory as the most robust description of reproducible experiments

Hans De Raedt<sup>a</sup>, Mikhail I. Katsnelson<sup>b</sup>, Kristel Michielsen<sup>c,d,\*</sup>

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

Hans De Raedt<sup>a</sup>, Mikhail I. Katsnelson<sup>b</sup>, Hylke C. Donker<sup>b</sup>, Kristel Michielsen<sup>c,d,\*</sup>

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

H.C. Donker<sup>a,\*</sup>, M.I. Katsnelson<sup>a</sup>, H. De Raedt<sup>b</sup>, K. Michielsen<sup>c</sup>

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

PHILOSOPHICAL TRANSACTIONS A

H. De Raedt<sup>1</sup>, M. I. Katsnelson<sup>2</sup> and K. Michielsen<sup>3,4</sup>

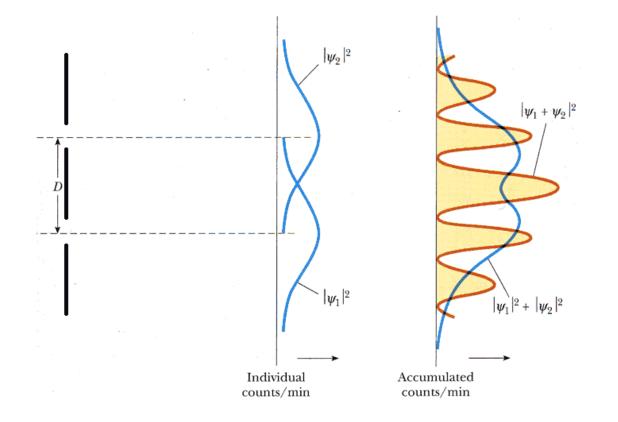
Annals of Physics 347 (2014) 45-73

Annals of Physics 359 (2015) 166-186

Annals of Physics 372 (2016) 74-82

**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. Microworld: waves are corpuscles, corpuscles are waves

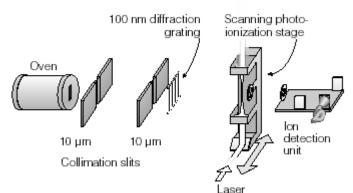
Einstein, 1905 – for light (photons) L. de Broglie, 1924 – electrons and other microparticles



#### Universal property of matter

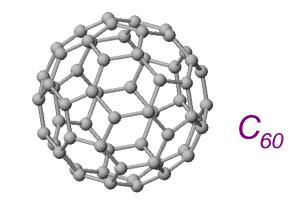
#### Wave—particle duality of C<sub>60</sub> molecules

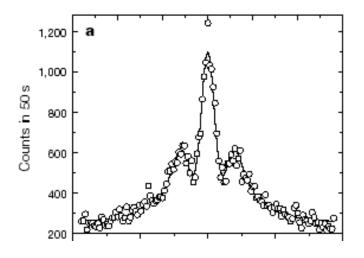
Markus Arndt, Olaf Nairz, Julian Vos-Andreae, Claudia Keller, Gerbrand van der Zouw & Anton Zeilinger



#### Matter waves for $C_{60}$ molecules

NATURE | VOL 401 | 14 OCTOBER 1999 |





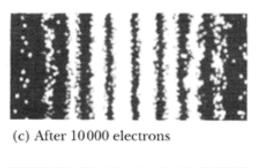
Electrons are particles (you cannot see half of electron) but moves along *all* possible directions (interference)

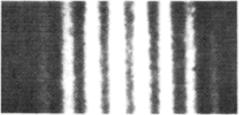


(a) After 28 electrons



(b) After 1000 electrons

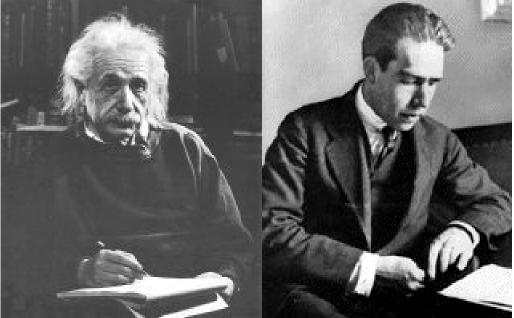




We cannot describe individual events, individual spots seem to be completely random, but ensemble of the spots forms regular interference fridges

Randomness in the foundations of physics?!





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

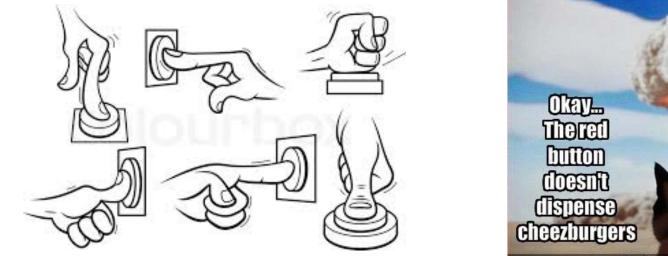
The limits of my language mean the limits of my world (Ludwig Wittgenstein)



## 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

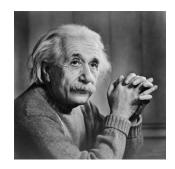
Knowledge begins, so to speak, in the middle, and leads into the unknown - both when moving upward, and when there is a downward movement. Our goal is to gradually dissipate the darkness in both directions, and the absolute foundation - this huge elephant carrying on his mighty back the tower of truth - 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?!

## 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.



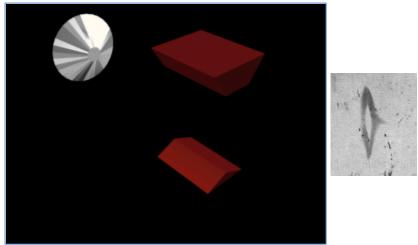
\*A. Petersen, "The philosophy of Niels Bohr," Bulletin of the Atomic Scientists 19, 8 – 14 (1963).

# Main message of this talk

- Logical inference applied to experiments for which
  - 1. There is uncertainty about each individual event
  - 2. The frequencies of observed events are robust with respect to small changes in the conditions
- → Basic equations of quantum theory
- Not an interpretation of quantum theory
- Derivation based on elementary principles of human reasoning and perception

#### Stern-Gerlach experiment

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

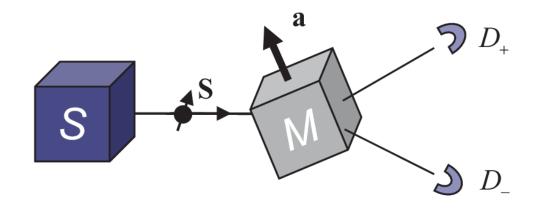


 Inference from the data: directional quantization Idealization  $a \rightarrow D_+$   $s \rightarrow D_+$  $D_-$ 

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

#### Idealized Stern-Gerlach experiment

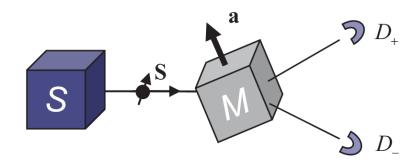
• Event = click of detector D<sub>+</sub> or (exclusive) D<sub>-</sub>



- There is uncertainty about each event
  - We do not know how to predict an event with certainty

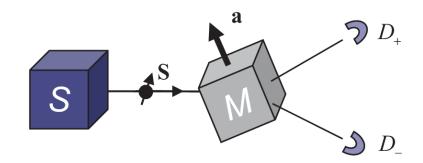
## Some reasonable assumptions (1)

- 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



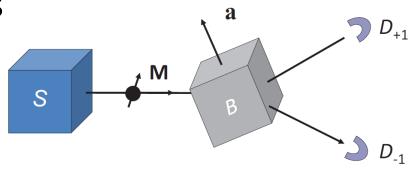
## Some reasonable assumptions (2)

- 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
  - $-x=+1 \Leftrightarrow D_+$  clicks
  - $-x=-1 \Leftrightarrow D_{-}$ clicks
  - $\mathbf{M} \Leftrightarrow$  the value of  $\mathbf{M}$  is  $\mathbf{M}$
  - 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 | M,a,Z) between 0 and 1 to express our expectation that detector D<sub>+</sub> or (exclusive) D<sub>-</sub> will click and want to derive, not postulate, P(x | M,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

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

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

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

- 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

- 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

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

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

Different events are logically independent:

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

 $\lambda T$ 

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

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

#### How to express robustness?

- Hypothesis  $H_0$ : given  $\theta$  we observe  $n_+$  and  $n_-$
- Hypothesis  $H_1$ : given  $\theta + \varepsilon$  we observe  $n_1$  and  $n_2$
- 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  $\theta \rightarrow$  we should minimize, in absolute value, the coefficients of  $\varepsilon$ ,  $\varepsilon^2$ ,...

Remove dependence on 
$$\epsilon$$
 (1)  

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

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

- Removes the 1<sup>st</sup> and 3<sup>rd</sup> 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 
$$\epsilon$$
 (2)  

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

• Minimizing the  $2^{nd}$  term (Fisher information) for all possible (small)  $\epsilon$  and  $\theta$ 

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

$$s \longrightarrow M$$

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

• 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  $\theta$  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

#### Separation procedure

Dataset in SG experiment:  $\mathscr{D} = \{x_1, \ldots, x_N \mid x_i = \pm 1, i = 1, \ldots, N\},\$ 

*N* is the total number of recorded events.

 $N(\pm 1 | \mathbf{a}, \mathbf{M}, Z)$  of outcomes with  $x = \pm 1$  ( $N = N(+1 | \mathbf{a}, \mathbf{M}, Z) + N(-1 | \mathbf{a}, \mathbf{M}, Z)$ )

$$\langle x \rangle = \frac{1}{N} \sum_{x=\pm 1} xN(x \mid \mathbf{a}, \mathbf{M}, Z) \equiv \sum_{x=\pm 1} xf(x \mid \mathbf{a}, \mathbf{M}, Z)$$

Rotational invarience: a crucial physical requirement

$$f(x \mid \mathbf{a}, \mathbf{M}, Z) = f(x \mid \mathbf{a} \cdot \mathbf{M}, Z)$$

Depends only on the angle  $\theta$ 

#### Separation procedure II

Presentation of measurement results in vector/matrix form

 $\mathbf{x} = (+1, -1)^{\mathrm{T}}$   $\mathbf{f} = (f(+1 | \mathbf{a}, \mathbf{M}, Z), f(-1 | \mathbf{a}, \mathbf{M}, Z))^{\mathrm{T}}$ 

 $\langle x \rangle = \mathbf{x}^{\mathrm{T}} \cdot \mathbf{f} = \mathrm{Tr} \, \mathbf{x}^{\mathrm{T}} \mathbf{f} = \mathrm{Tr} \, \mathbf{f} \mathbf{x}^{\mathrm{T}}$ 

When we rotate measurement device we want to separate the data on particle and the data on device for any angle  $\theta$ .

It cannot be done with vectors but can be done with matrices dependent on pairs of outcomes



Heisenberg argument: we cannot probe atomic states but only transitions between two atomic states – therefore two-index objects!

#### Separation procedure III

$$\langle x \rangle = \operatorname{Tr} F X = \operatorname{Tr} \hat{\rho} \hat{X}$$
  $\hat{\rho} = \frac{\mathbb{1} + \rho \cdot \sigma}{2}$  and  $\hat{X} = u_0 \mathbb{1} + \mathbf{u} \cdot \sigma$ 

The first object (density matrix) depends on orientation of particles, the second – on the measurement device

Logical inference results can be represented in this way

$$\hat{\rho} = \frac{(\mathbb{1} + \mathbf{M} \cdot \boldsymbol{\sigma})}{2}$$
 and  $\hat{X} = \mathbf{a} \cdot \boldsymbol{\sigma}$ 

Projection operator property:  $\hat{\rho}^2 = \hat{\rho}$ 

$$\hat{\rho} = |\Psi\rangle\langle\Psi|, \quad |\Psi\rangle = a_{\uparrow}|\uparrow\rangle + a_{\downarrow}|\downarrow\rangle$$

Existence of "wave function" is derived (also, for EPRB experiment)

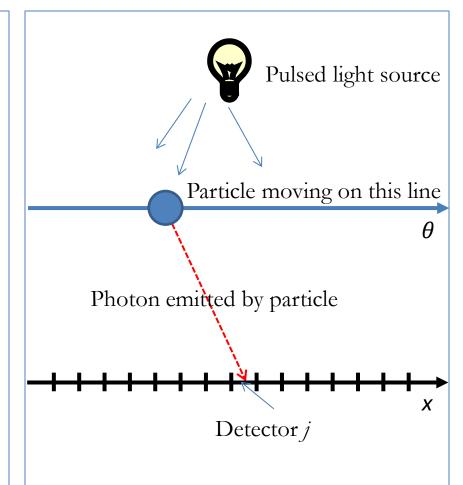
# Derivation of basic results of quantum theory by logical inference

- 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
  - Minimize functional → equation of quantum theory when applied to experiments in which
    - i. There is uncertainty about each event
    - ii. The conditions are uncertain
    - iii. 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  $\theta$  activates the detector at position  $x : P(x | \theta, Z)$



#### Robustness

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

 $P(x \mid \theta, Z) = P(x + \zeta \mid \theta + \zeta, Z)$ ;  $\zeta$  arbitrary

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

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

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

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

• If there is "known" uncertainty

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

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

 $-\lambda$  = 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\*

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



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

• Minimizing with respect to  $\psi(x|\theta, Z)$  yields

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

→ 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  $\tau = 1, ..., M$ 

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

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

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

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

Logical independence of events:

$$P(\mathcal{D}|\boldsymbol{\theta}_1,\ldots,\boldsymbol{\theta}_M,N,Z) = N! \prod_{\tau=1}^M \prod_{\boldsymbol{j}\in [-L^d,L^d]} \frac{P(\boldsymbol{j}|\boldsymbol{\theta}_{\tau},\tau,Z)^{k_{\boldsymbol{j},\tau}}}{k_{\boldsymbol{j},\tau}!}$$

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

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

and, by using the Cauchy-Schwarz inequality, that

$$\begin{aligned} \mathsf{Ev} &\leq \sum_{j,\tau} \left( \sum_{i=1}^{d} \epsilon_{i,\tau}^{2} \right) \left( \sum_{i=1}^{d} \frac{1}{P(\boldsymbol{j}|\boldsymbol{\theta}_{\tau},\tau,Z)} \left( \frac{\partial P(\boldsymbol{j}|\boldsymbol{\theta}_{\tau},\tau,Z)}{\partial \theta_{i}} \right)^{2} \right) \qquad \widehat{\boldsymbol{\epsilon}}^{2} = \max_{i,\tau} \epsilon_{i,\tau}^{2} \\ &\leq d\widehat{\boldsymbol{\epsilon}}^{2} \sum_{\boldsymbol{j},\tau} \sum_{i=1}^{d} \frac{1}{P(\boldsymbol{j}|\boldsymbol{\theta}_{\tau},\tau,Z)} \left( \frac{\partial P(\boldsymbol{j}|\boldsymbol{\theta}_{\tau},\tau,Z)}{\partial \theta_{i}} \right)^{2}, \end{aligned}$$

#### Time-dependent case III

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

Taking into account homogeneity of space; continuum limit:

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

Hamilton – Jacobi equations:

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

#### Time-dependent case IV

 $\lambda = 4/\hbar^2$ 

Minimizing functional:

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

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

Equivalent functional for minimization:

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

J

#### 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 + $2\pi\hbar$  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!

#### Next steps

Pauli equation for nonrelativistic particle with spin – done

2. Klein-Gordon equation for relativistic particle, no spin – done

3. Dirac equation for relativistc particle with spin – in progress

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

# Thank you