Title: A Unification of Quantum and Classical Mechanics through Ehrenfest Theorems

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Abstract: We present a quantization method based on theEhrenfest theorem embedded in an extended algebraic structure capableof consistently describing hybrid quantum-classical systems, where thestandard quantum and classical mechanics are two limiting cases. TheWigner phase space formulation and the Schordinger equation are foundto be two alternative representations of the quantum case while theKoopman-von Neumann equation is the corresponding classicalcounterpart. Moreover, the developed quantization procedure isgeneralized to describe open systems, quantum/classical field theoriesand relativistic mechanics where new dynamical equations appear,shedding new light on important practical problems such asunderstanding of the quantum/classical transition and modeling ofmesoscopic systems.

Related references: arXiv:1105.4014, arXiv:1112.3679, arXiv:1107.5139

The Quantum-Classical Reconciliation is needed for describing

- Photosynthesis
- Nano-scale systems
- Large molecular complexes
- Mesoscopic physics

Outline

- Approach
- Rederivation of Nonrelativistic Classical Mechanics
- Rederivation of Nonrelativistic Quantum Mechanics
- Derivation of Unified Mechanics
- So what?

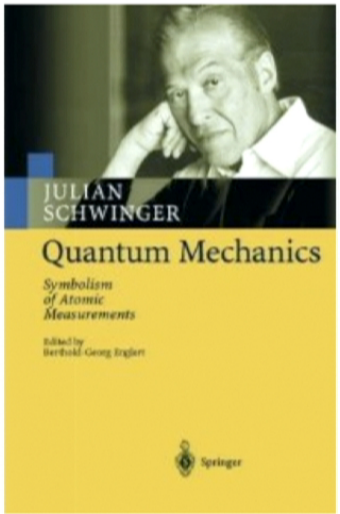
Operational Approach to Quantum Mechanics

The source of inspiration:

J. Schwinger,

"Quantum Mechanics: Symbolism of Atomic Measurements"

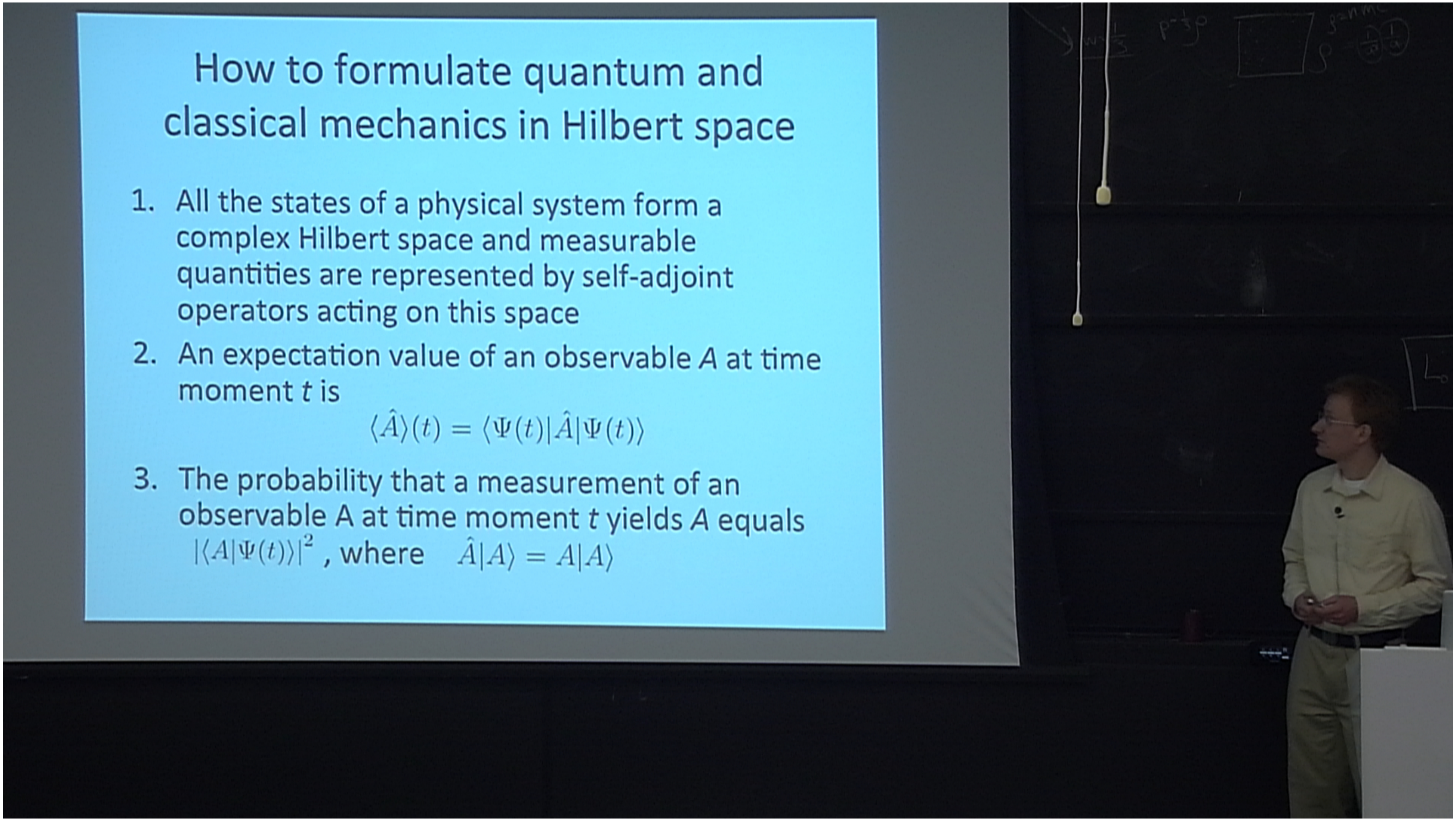
(Springer, 2003)



Modern operational approaches: L. Hardy, S. Abramsky, B. Coecke, G. Chiribella, G. M. D'Ariano, and P. Perinotti, C. A. Fuchs, ...

Approach

- *Any* physical theory is a symbolic representation of experimental evidences supporting it
- The operational approach can be applied to quantum as well as classical mechanics
- The Hilbert space is a very general and mathematically rich symbolism (i.e., formalism)


How to formulate quantum and classical mechanics in Hilbert space
1. All the states of a physical system form a complex Hilbert space and measurable quantities are represented by self-adjoint operators acting on this space
2. An expectation value of an observable *A* at time moment *t* is
$\langle \hat{A} \rangle (t) = \langle \Psi(t) | \hat{A} | \Psi(t) \rangle$
3. The probability that a measurement of an observable A at time moment *t* yields *A* equals $|\langle A | \Psi(t) \rangle|^2$, where $\hat{A}|A\rangle = A|A\rangle$

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Classical kinematics

The commutation relation

$$[\hat{x}, \hat{p}] = 0$$

symbolizes the experimental fact that the order in a sequence of measurements *does not* matter,

$$x_1\ p_1\ x_2\ p_2 = p_{1'}\ x_{1'}\ p_{2'}\ x_{2'}$$

i.e.,

$$x_1 = x_{1'} \quad p_1 = p_{1'} \quad x_2 = x_{2'} \quad p_2 = p_{2'}$$

Derivation of the Liouville equation from the Ehrenfest theorems

Newton's Equations for Ensemble Averages

$$m\frac{d}{dt}\langle\Psi(t)|\hat{x}|\Psi(t)\rangle = \langle\Psi(t)|\hat{p}|\Psi(t)\rangle$$

$$\frac{d}{dt}\langle\Psi(t)|\hat{p}|\Psi(t)\rangle = \langle\Psi(t)| - U'(\hat{x})|\Psi(t)\rangle$$

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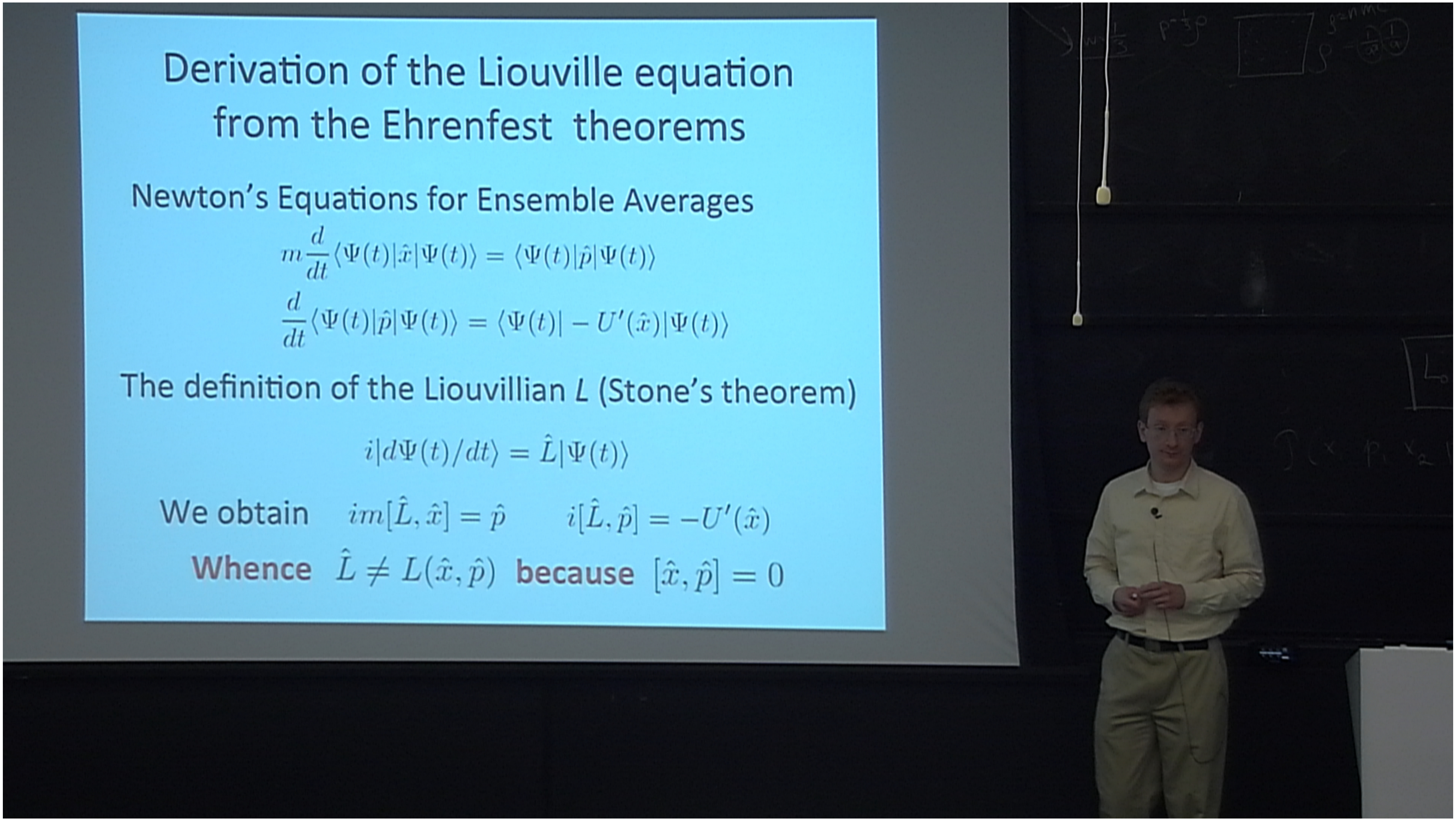
The definition of the Liouvillian *L* (Stone's theorem)

$$i|d\Psi(t)/dt\rangle = \hat{L}|\Psi(t)\rangle$$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We obtain $im[\hat{L},\hat{x}] = \hat{p}$ $i[\hat{L},\hat{p}] = -U'(\hat{x})$
Whence $\hat{L} \neq L(\hat{x},\hat{p})$ because $[\hat{x},\hat{p}] = 0$

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We must introduce auxiliary operators

$$[\hat{x}, \hat{\lambda}_x] = [\hat{p}, \hat{\lambda}_p] = i$$

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The secret ingredient:

Theorem For any function of operators

$$[f(\hat{A}_1, \ldots, \hat{A}_n), \hat{B}] = \sum_{k=1}^{n} [\hat{A}_k, \hat{B}] f'_{\hat{A}_k}(\hat{A}_1, \ldots, \hat{A}_n)$$

If $[\hat{A}_k, \hat{B}]$ are complex numbers.

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Derivation of the Liouville equation from the Ehrenfest theorems

Assuming that $\hat{L} = L(\hat{x}, \hat{\lambda}_x, \hat{p}, \hat{\lambda}_p)$

By means of *the secret ingredient*, we go from

$$im[\hat{L}, \hat{x}] = \hat{p} \qquad i[\hat{L}, \hat{p}] = -U'(\hat{x})$$

to the system of differential equations

$$mL'_{\lambda_x}(x, \lambda_x, p, \lambda_p) = p \qquad L'_{\lambda_p}(x, \lambda_x, p, \lambda_p) = -U'(x)$$

Derivation of the Liouville equation from the Ehrenfest theorems

The Liouville equation $i|d\Psi(t)/dt\rangle = \hat{L}|\Psi(t)\rangle$ reads in the *px* – representation

$$\hat{p} = p \qquad \hat{\lambda}_p = -i\frac{\partial}{\partial p} \qquad \hat{x} = x \qquad \hat{\lambda}_x = -i\frac{\partial}{\partial x}$$

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$$i\frac{\partial}{\partial t}\langle p\, x|\Psi(t)\rangle = \left[-i\frac{p}{m}\frac{\partial}{\partial x} + iU'(x)\frac{\partial}{\partial p} + f(x,p)\right]\langle p\, x|\Psi(t)\rangle$$

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The probability density $\rho(x,p) = |\langle p\, x|\Psi(t)\rangle|^2$ satisfy

$$\frac{\partial}{\partial t}\rho(x,p) = \left[-\frac{p}{m}\frac{\partial}{\partial x} + U'(x)\frac{\partial}{\partial p}\right]\rho(x,p)$$

This is the text-book Liouville equation

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The general form of the Liouvillian reads:

$$\hat{L} = \hat{p}\hat{\lambda}_x/m - U'(\hat{x})\hat{\lambda}_p$$
$$+ \text{ any real function of } \hat{x} \text{ and } \hat{p}$$

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The Hilbert space reformulation of classical mechanics is known as

The Koopman-von Neumann class. mechanics

B. O. Koopman, PNAS USA **17**, 315 (1931)

J. von Neumann, Ann. Math. **33**, 587 (1932)

For review see

D. Mauro *"Topics in Koopman-von Neumann Theory"* PhD thesis [arXiv:quant-ph/0301172]

Derivation of the Schrödinger equation from the Ehrenfest theorems

The Ehrenfest theorems

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The definition of the Hamiltonian *H*

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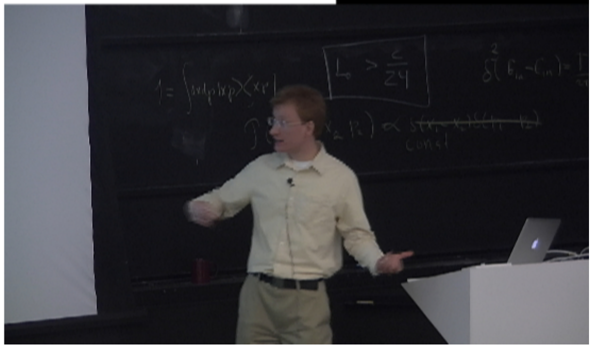

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Contrary to class. mechanics, it is OK to assume

$\hat{H} = H(\hat{x}, \hat{p})$ **because** $[\hat{x}, \hat{p}] = i\hbar$

Derivation of the Schrödinger equation from the Ehrenfest theorems

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The secret ingredient leads to

$$mH'_p(x,p) = p \qquad H'_x(x,p) = U'(x)$$

$$\hat{H} = \frac{\hat{p}^2}{2m} + U(\hat{x})$$

(note no ambiguities!)

Ehrenfest quantization: Classical Mechanics

Ehrenfest theorems

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↓

Definition of Liouvillian *L* (Stone's theorem)

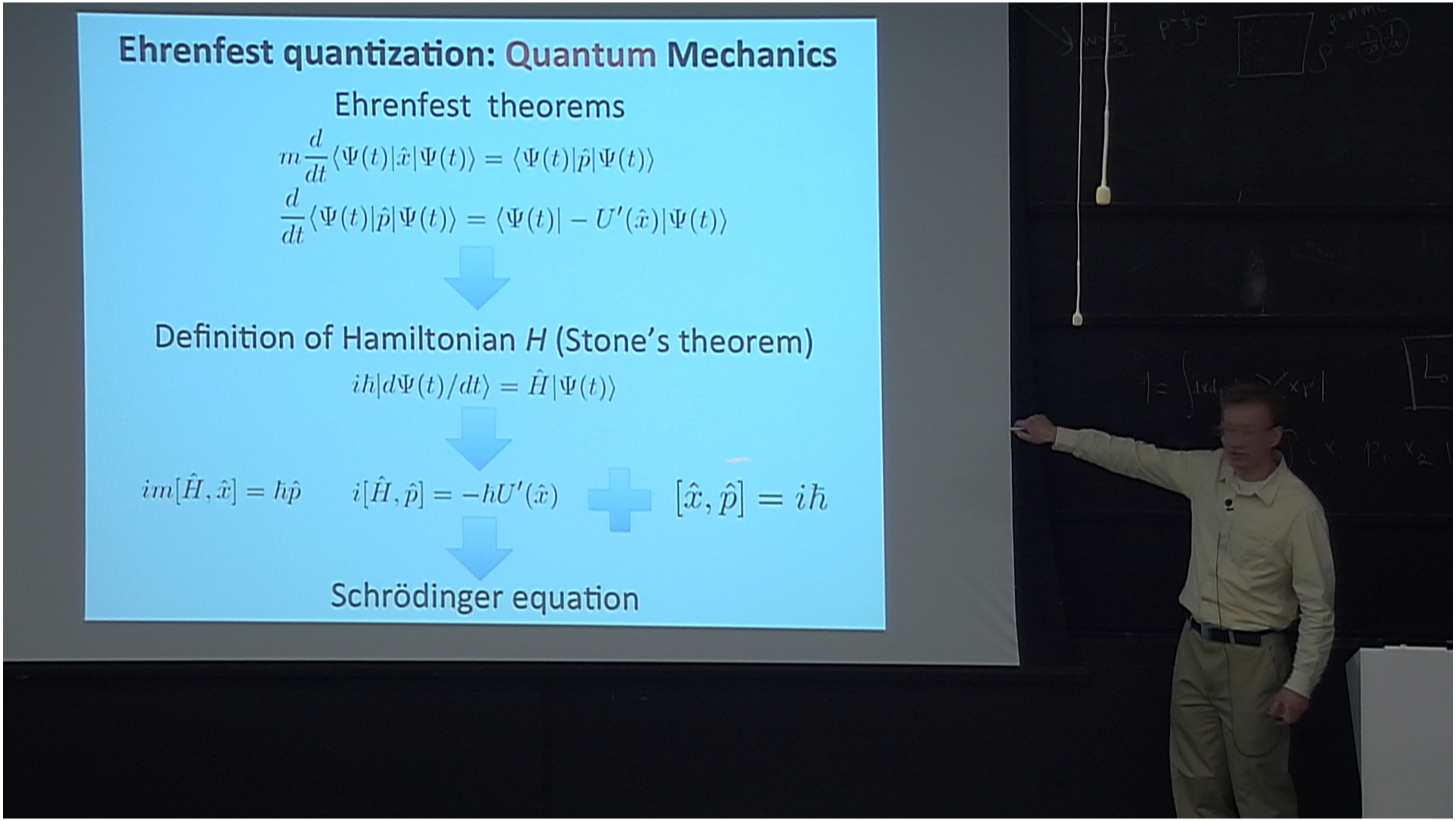
$$i|d\Psi(t)/dt\rangle = \hat{L}|\Psi(t)\rangle$$

↓

$$im[\hat{L},\hat{x}] = \hat{p} \qquad i[\hat{L},\hat{p}] = -U'(\hat{x}) \qquad + \qquad [\hat{x},\hat{p}] = 0$$

↓

Liouville equation


Ehrenfest quantization: Quantum Mechanics
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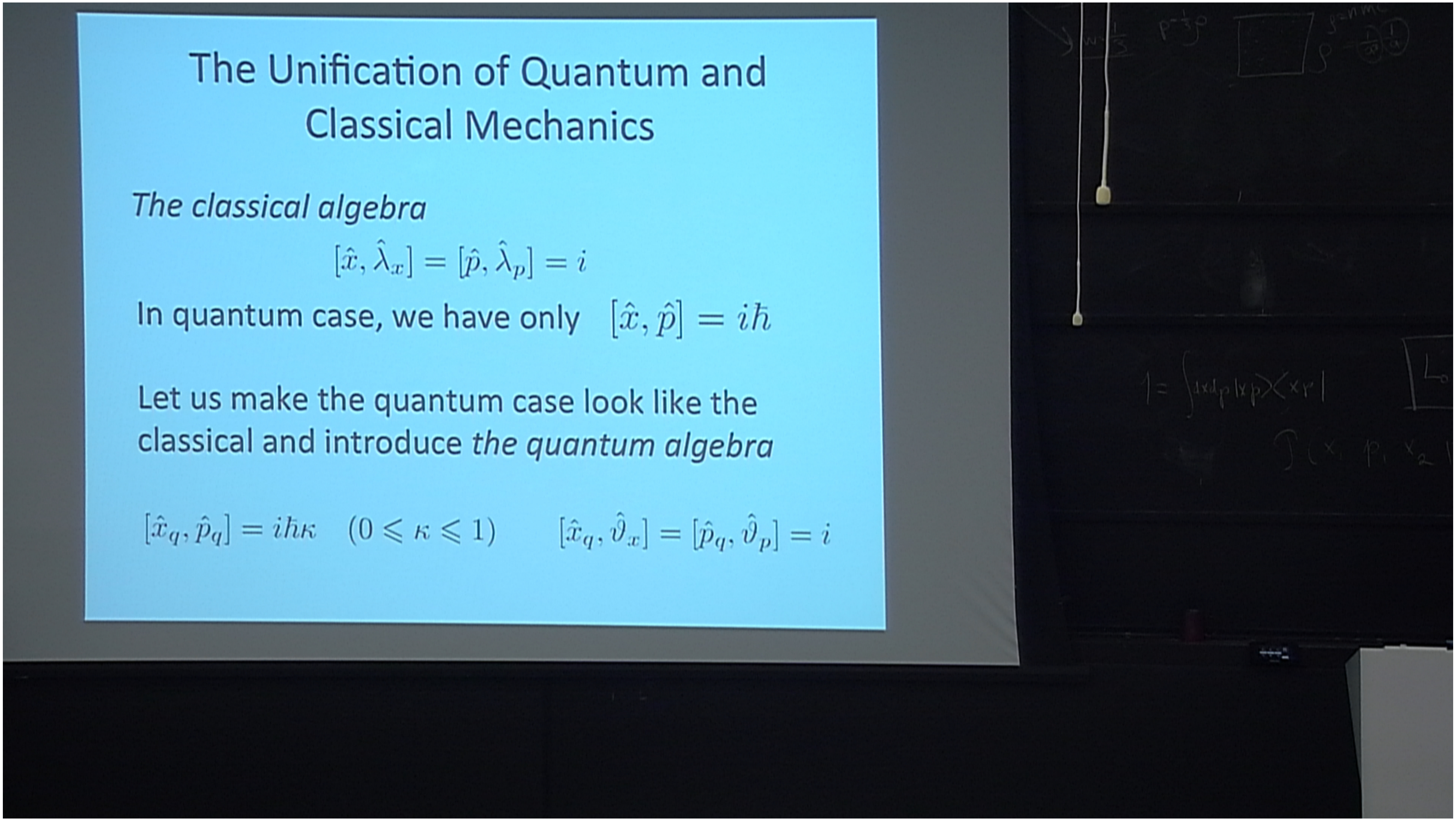
Definition of Hamiltonian H (Stone's theorem)
$i\hbar|d\Psi(t)/dt\rangle = \hat{H}|\Psi(t)\rangle$
$im[\hat{H},\hat{x}] = \hbar\hat{p}$
$i[\hat{H},\hat{p}] = -\hbar U'(\hat{x})$
$[\hat{x},\hat{p}] = i\hbar$
Schrödinger equation


The Unification of Quantum and Classical Mechanics
The classical algebra
$[\hat{x}, \hat{\lambda}_x] = [\hat{p}, \hat{\lambda}_p] = i$
In quantum case, we have only $[\hat{x}, \hat{p}] = i\hbar$
Let us make the quantum case look like the classical and introduce the quantum algebra
$[\hat{x}_q, \hat{p}_q] = i\hbar\kappa \quad (0 \leqslant \kappa \leqslant 1) \qquad [\hat{x}_q, \hat{\vartheta}_x] = [\hat{p}_q, \hat{\vartheta}_p] = i$

The Unification of Quantum and Classical Mechanics

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The Unification of Quantum and Classical Mechanics

From the Ehrenfest theorems

$$m\frac{d}{dt}\langle\Psi(t)|\hat{x}_q|\Psi(t)\rangle = \langle\Psi(t)|\hat{p}_q|\Psi(t)\rangle$$

$$\frac{d}{dt}\langle\Psi(t)|\hat{p}_q|\Psi(t)\rangle = \langle\Psi(t)| - U'(\hat{x}_q)|\Psi(t)\rangle$$

and $i\hbar|d\Psi(t)/dt\rangle = \hat{\mathcal{H}}|\Psi(t)\rangle$ where $\hat{\mathcal{H}} = \mathcal{H}(\hat{x}_q, \hat{p}_q, \hat{\vartheta}_x, \hat{\vartheta}_p)$

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we get

any function

$$\hat{\mathcal{H}} = \frac{1}{\kappa}\left[\frac{\hat{p}_q^2}{2m} + U(\hat{x}_q)\right] + F\left(\hat{p}_q - \hbar\kappa\hat{\vartheta}_x, \hat{x}_q + \hbar\kappa\hat{\vartheta}_p\right)$$

The Unification of Quantum and Classical Mechanics

However, the quantum and classical algebras are the same! There exist infinitely many linear isomorphisms between the two algebras. For example,

$$\hat{x}_q = \hat{x} - \hbar\kappa\hat{\lambda}_p/2 \qquad \hat{p}_q = \hat{p} + \hbar\kappa\hat{\lambda}_x/2$$

$$\hat{\vartheta}_x = \hat{\lambda}_x \qquad \hat{\vartheta}_p = \hat{\lambda}_p$$

Transitions between Quantum and Classical Mechanics

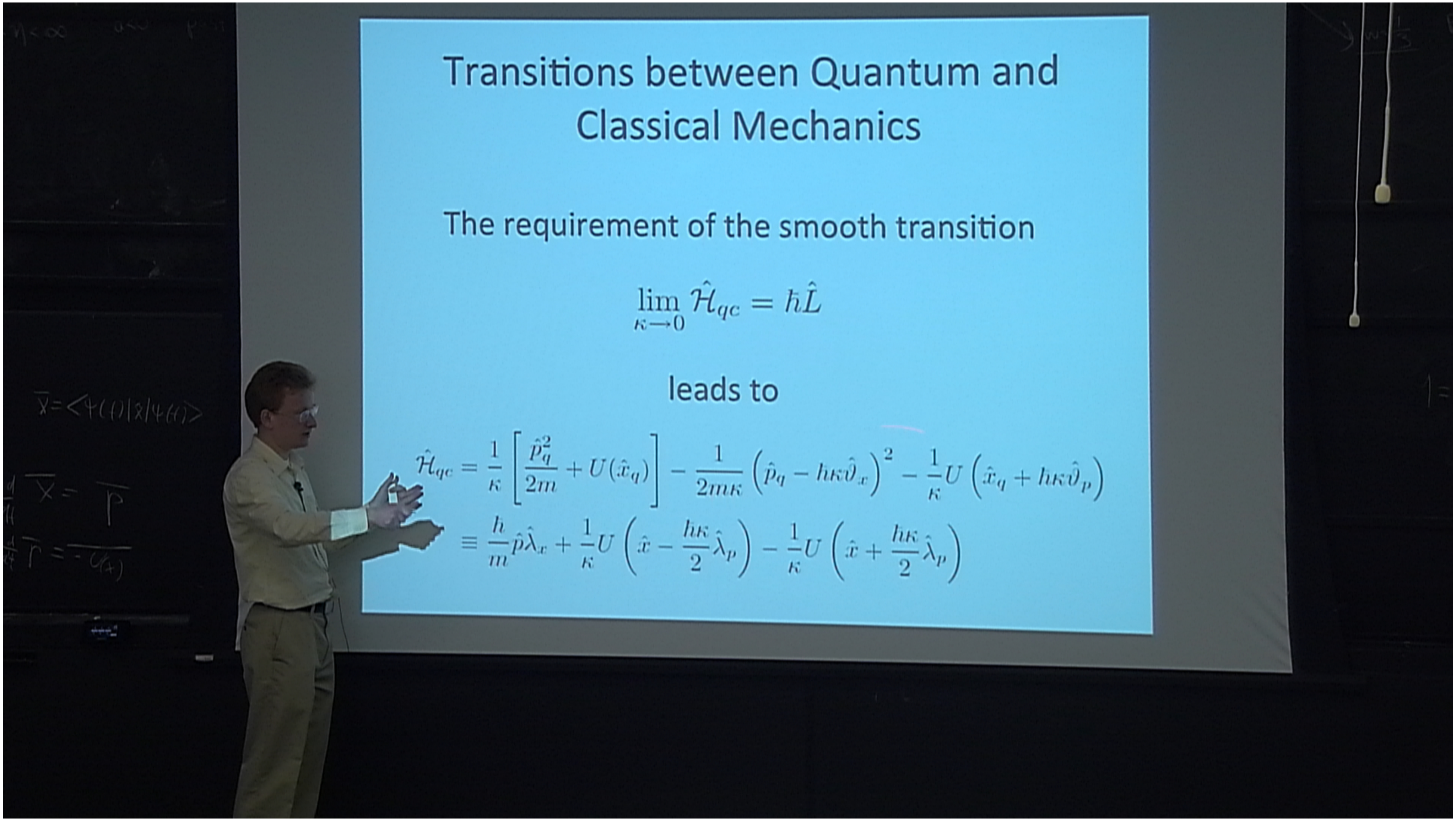
The requirement of the smooth transition

$$\lim_{\kappa \longrightarrow 0} \hat{\mathcal{H}}_{qc} = \hbar \hat{L}$$

leads to

$$\hat{\mathcal{H}}_{qc} = \frac{1}{\kappa}\left[\frac{\hat{p}_q^2}{2m} + U(\hat{x}_q)\right] - \frac{1}{2m\kappa}\left(\hat{p}_q - \hbar\kappa\hat{\vartheta}_x\right)^2 - \frac{1}{\kappa}U\left(\hat{x}_q + \hbar\kappa\hat{\vartheta}_p\right)$$

$$\equiv \frac{\hbar}{m}\hat{p}\hat{\lambda}_x + \frac{1}{\kappa}U\left(\hat{x} - \frac{\hbar\kappa}{2}\hat{\lambda}_p\right) - \frac{1}{\kappa}U\left(\hat{x} + \frac{\hbar\kappa}{2}\hat{\lambda}_p\right)$$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The Wigner Quasi-probability Distribution Formulation as a Special Representation of this Formalism

The solution of $i\hbar|d\Psi_\kappa(t)/dt\rangle = \hat{\mathcal{H}}_{qc}|\Psi_\kappa(t)\rangle$

in the *px* – representation

$$\frac{\partial}{\partial t}\rho(x,p) = \left[-\frac{p}{m}\frac{\partial}{\partial x} + U'(x)\frac{\partial}{\partial p}\right]\rho(x,p)$$

The Wigner Quasi-probability Distribution Formulation as a Special Representation of this Formalism

The solution of $i\hbar|d\Psi_\kappa(t)/dt\rangle = \hat{\mathcal{H}}_{qc}|\Psi_\kappa(t)\rangle$

in the *px* – representation coincides with the Wigner quasi-probability distribution

$$W(p,x;t) = \langle p\,x|\Psi_\kappa(t)\rangle$$
$$= \int \frac{d\lambda_p}{\sqrt{2\pi}} \Psi\left(x - \hbar\kappa\lambda_p/2, t\right) \Psi^*\left(x + \hbar\kappa\lambda_p/2, t\right) e^{ip\lambda_p}$$

where Ψ is the solution of the Schrödinger Eq.

Remarks on the Unification

- The Wigner formulation is the only one consistently reconciling quantum and classical mechanics
- Our representation of the Wigner function allows for an effective numerical implementation
- The Wigner phase-space distribution maps a quantum mechanical wave function into a Koopman-von Neumann classical wave function (not a classical phase-space distribution!)

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A Wigner distribution as a Koopman-von Neumann wave function

if $W(p,x;t) := \int \frac{d\lambda_p}{2\pi} \Psi\left(x - \frac{\hbar\lambda_p}{2};t\right) \Psi^*\left(x + \frac{\hbar\lambda_p}{2};t\right) e^{ip\lambda_p}$

then $1 = \int dxdpW(p,x;t) = 2\pi\hbar \int dxdp\,|W(p,x;t)|^2$

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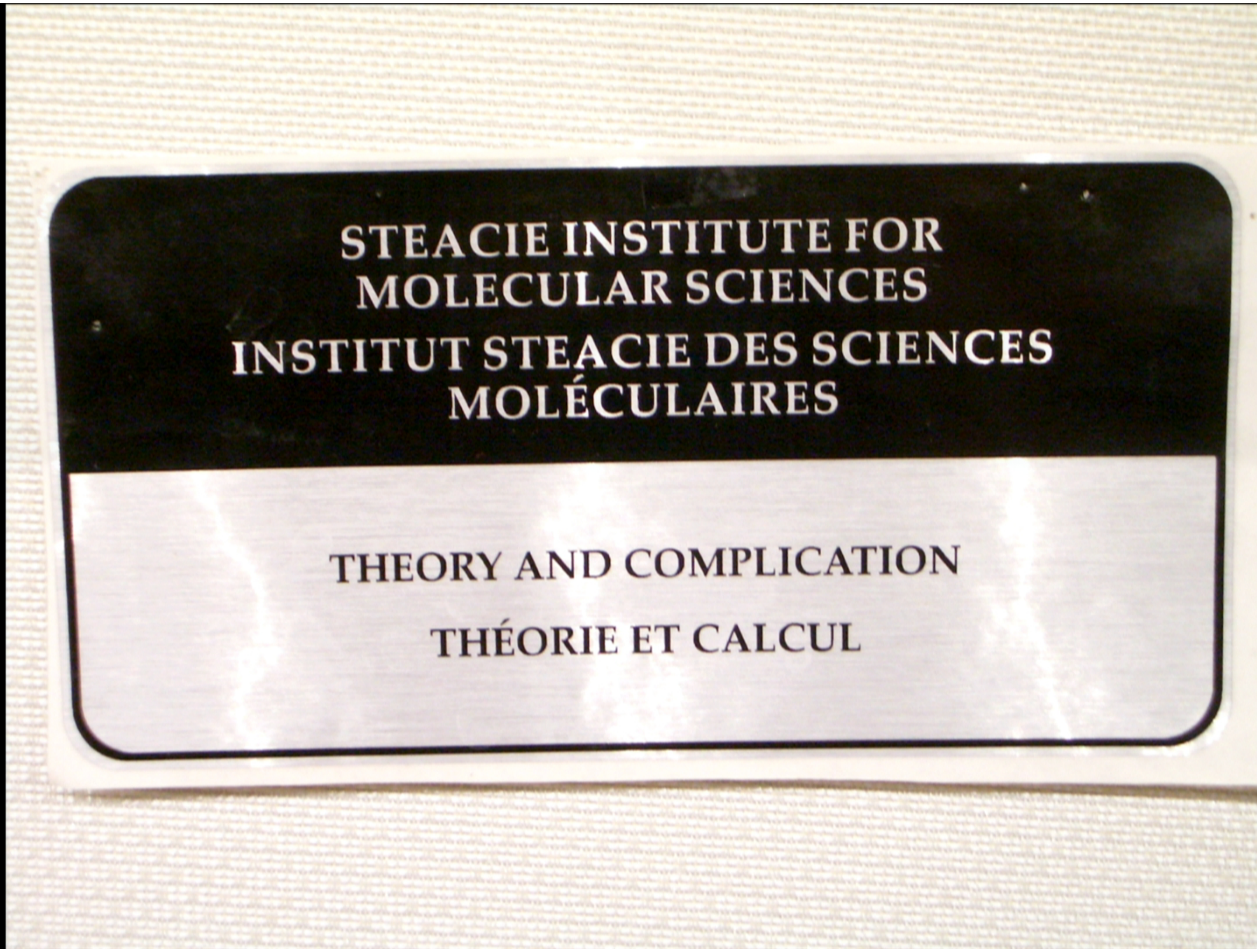
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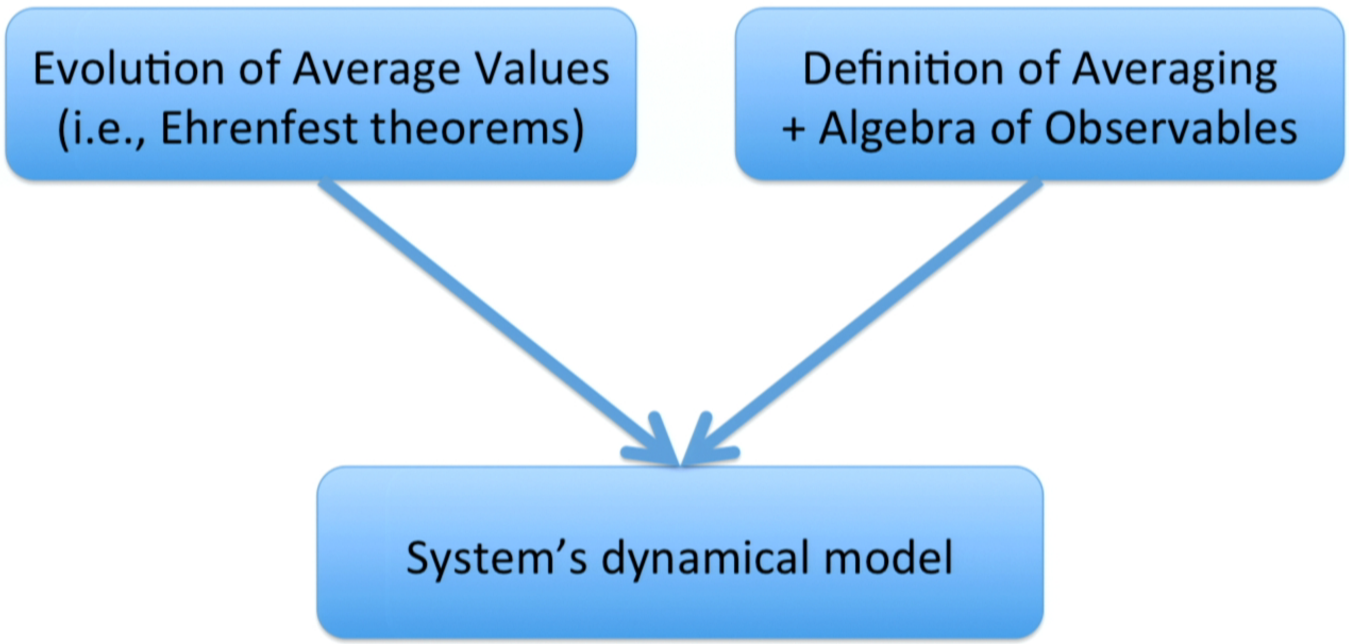
The Paradigm of the Ehrenfest Quantization



The Impact of the Ehrenfest Quantization

- Allow to construct consistent hybrid systems
- Revise the theories of open quantum and classical systems
- Reformulate quantum and classical field theories
- Develop relativistic classical and quantum mechanics (e.g., Renan’s spinorial classical and quantum equations)
- Quantization in curvilinear-coordinates
- Derive new physical theories
- Offer a new methodological perspective