Quantum mechanics via Schrödinger's problem, Mass transportation and back

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Joint work with Q. Huang.

1. Brief summary of (Von Neumann's) QM in general ∞ dim. separable Hilbert space, $< \cdot | \cdot >_2$.

In complex Hilbert space $\mathcal{H}(M)$, a ray $= \{\alpha\Psi, \Psi \in \mathcal{H}, \|\Psi\| = 1, \alpha \in \mathbb{C}, |\alpha| = 1\}$ = quantum (pure) state of system.

Ex. Ψ = Schrödinger's "wave function".

To each classical $a(q, p)$ observable $\longleftrightarrow$ unique s.a. densely defined self-adjoint operator A in $\mathcal{H}$.

1. a) Quantum static

For Ψ state at t_0, A with spectral family $E^A(\lambda)$ of orthogonal projections, the prob. that a measurement of A is $\leq \lambda$ is

$$< \Psi|E^A(\lambda)\Psi >= \|E^A(\lambda)\Psi\|^2 \Rightarrow \text{ if } \Delta =]\lambda_1, \lambda_2], E^A(\Delta) = E^A(\lambda_2) - E^A(\lambda_1)$$

$$\Pr_\Psi\{ \text{ value of } A \in \Delta\} = \|E^A(\lambda)\Psi\|^2 \neq 0 \text{ if } \Delta \subset \sigma_A$$

Expectation of A in Ψ : $< \Psi|A\Psi >= \int \lambda \underbrace{< \Psi|dE^A(\lambda)\Psi >}_{\text{"Prob." measure for } A}$ on $\mathcal{D}_A \subset \mathcal{H}$

Position $Q : \mathcal{D}_Q \to \mathcal{H} = L^2(\mathbb{R})$

$$\Psi(q) \to q\Psi(q)$$

$E^Q(\lambda) = 1_{]-\infty,\lambda]}(q)$ heuristic $E^Q(\lambda)\Psi = \int_{-\infty}^{\lambda} \Psi(x)\delta(q-x)dx$

$\|E^Q(\Delta)\Psi\|^2 = \int_\Delta |\Psi(q)|^2 dq$, Spectrum $\sigma_Q = \mathbb{R}$,

$< Q >_\Psi = \int_\mathbb{R} q|\Psi(q)|^2 dq$

Momentum $P : \mathcal{D}_P \to L^2(\mathbb{R})$, Fourier transform of $\Psi(q) \to$

$$\Psi(q) \to -i\hbar\frac{\partial}{\partial q}\Psi(q)$$

$< P >_\Psi = \int_\mathbb{R} \Big(-i\hbar\nabla \log \Psi(q)\Big)|\Psi(q)|^2 dq$, $\sigma_P = \mathbb{R}$

Hamiltonian $H = \frac{1}{2}P^2 + V(Q) = -\frac{\hbar^2}{2}\Delta + V = H_0 + V$.
$\frac{i}{\hbar}[H, Q] = -i\hbar\nabla = P \quad , \quad \frac{d}{dt} < Q >_\Psi = < P >_\Psi$

also $\frac{d}{dt} < P >_\Psi = < -\nabla V >_\Psi$, not $-\nabla V(< Q >_\Psi)$!

1 b) Quantum Dynamics

As in regular probability theory

$“\mathrm{Pr}"_\Psi \{\text{value of } A \in \Delta\} = < \chi_\Delta(A) >_\Psi$

For given observable A , $A(t) = e^{it\frac{H}{\hbar}} A e^{-it\frac{H}{\hbar}}$,

$\frac{d}{dt}A(t) = \frac{i}{\hbar}[H, A(t)], \qquad \Psi(t) = e^{-it\frac{H}{\hbar}}\Psi_0$, $\begin{cases} i\hbar\frac{\partial\Psi}{\partial t} = H\Psi \\ \Psi(0) = \Psi_0 \end{cases}$

$< A >_{\Psi(t)} = < A(t) >_{\Psi_0}$

Schrödinger Heisenberg

Conceptual difficulties

a) Meaning of $< \; | \; >_\Psi$?

$\nexists$ mathematical probabilities in Von Neumann axioms (He knew it. Did not like it.)

Where are (Feynman's) diffusions expected for H, with $(\Omega, \mathcal{P}_t, P_r)$?

For Q, "diffusion" Z_t s.t $\rho_t(dq) = \bar{\Psi}_t(q)\Psi_t(q)dq$? Proved inexistent : R. H. Cameron (1960).

NB : $< P >_{\Psi_t}$ suggests $\Big(-i\frac{\nabla\Psi_t}{\Psi_t}(q)\Big)$ as complex valued vector field (drift) of Z_t.

b) Quantization $\neq$ algorithm   Axiom 2 $(a \to A)$ too naïve.

Operator associated with $\forall\; a(q,p)$? Since Heisenberg's $[Q,P] = i\hbar$ ("Incompatible measurements" !) $\Rightarrow$ Different choices of $A(Q;P)$.

c) $\text{limit}_{\hbar\downarrow 0}$ Q.M. not trivial.
Ex. $\text{limit}_{\hbar\downarrow 0} P = 0$? Only $\lim_{\hbar\downarrow 0} < P >_{\Psi_t}$ is OK.

d) $\nexists$ quantum trajectories in space-time. For $h_0(q,p) = \frac{1}{2}p^2$,
$H_0 = -\frac{\hbar^2}{2}\Delta, Q(t) = Q + tP, P(t) = P$ but $[Q(t), Q(0)] = -i\hbar t$, $\forall t > 0$
$\rightarrow$ $\nexists$ space-time history ! $\rightarrow$ Surrealistic interpretations. $\nexists$ reality !

For same reason, $\nexists$ joint probability : natural candidate (Cf. Feynman) $\in \mathbb{C}$.

2) 1931-32 Schrödinger's problem of classical statistical physics

Motivation : Analogy with QM without ideological bias.

Brownian motion $=$ 25 years old in 1931. Tool of classical statistical physics, associated with $-\frac{\partial \eta^*}{\partial t} = H_0 \eta^*$ (Cauchy) $\eta^*_\chi(q,0) = \chi(q) > 0$ ("heat" !)

NB : $\forall V$ bounded below , sol. $\Psi_\chi(q,\tau) = (e^{-i\tau H}\chi)(q)$ after $\tau \to i\tau = t$ is $\eta^*_\chi(q,t)$ pointwise solution of heat eq. ("Euclidean" Schrödinger's eq.)

Mystery : All probabilistic results of quantum physics minimally consistent with regular QM are Euclidean. (Nelson's theory was not : Brownian $\neq$ sol. for $V = 0$)

Key Schrödinger's observation :

$$\bar{\Psi}_t(q)\Psi_t(q)dq \longrightarrow i\frac{\partial \Psi}{\partial t} = H_0\Psi$$

$$\searrow \quad -i\frac{\partial \bar{\Psi}}{\partial t} = H_0\bar{\Psi}$$

Quantum time-reversibility.

So: Formulate a parabolic problem whose solution is well def. probab. density : $\rho_t(dq) = \eta_t^*(q)\eta_t(q)dq$ for $0 < \eta_t$ s.t. $\frac{\partial \eta}{\partial t} = H_0\eta, t \in [s, u]$, $\eta_t^* > 0$, given $\eta(q, u) > 0$.

Result (with Q. Huang) : Stochastic geometric Lagrangian/Hamiltonian dynamics of well defined diffusion $X_t, s \leq t \leq u$, (called "Bernstein" for historical reasons), solving Schrödinger's problem.

Key ingredient

1933 Axiomatic foundations of Probab. Theory by Kolmogorov, analyst (with Chapman).

Dynamics = Cauchy problems, Ex. $\rho_s(dq)$, incompatible with Schrödinger's problem.

Probabilistic data : An Hamiltonian H , a joint density $M(dx, dz)$ at $\partial[s, u]$, containing all possible correlations between processes X_s, X_u with density $\{\rho_s(dx), \rho_u(dz)\}$ = Data of Schrödinger's probab.

Idea of probabilistic proof of existence

Origin : Feyman's PhD "transition amplitude"

$$\int\int \Psi_s(x) \underbrace{K(x, u-s, z)} \bar{\varphi}_u(z) dxdz =< \varphi_s | \Psi_s >_2 \ \in \mathbb{C} \ !$$

$$(e^{-\frac{i}{\hbar}(u-s)H}) = \int_{\Omega_x^z} e^{\frac{i}{\hbar} S_L[\omega(\cdot), u-s]} \mathcal{D}\omega$$

Euclidean version : $M(dx, dz) = \int\int \eta_s^*(x) \underbrace{h(x, u-s, z)}_{(e^{-\frac{1}{\hbar}(u-s)H})>0} \eta_u(z) dxdz$

Marginals of M $\begin{cases} \eta_s^*(x) \int h(x, u-s, z)\eta_u(z)dz = \rho_s(dx) \\ \eta_u(z) \int \eta_s^*(x)h(x, u-s, z)dx = \rho_u(dz) \end{cases}$ given Schrödinger's data.

Existence/uniqueness of $\eta_s^*, \eta_u > 0$ (A. Beurling, Ann. Math. 1960)
$\Rightarrow \quad \eta_t^*(q), \eta_t(q), \; \forall s \leq t \leq u$, i.e. $\rho_t(q)dq$.

Euclidean counterpart of
$< P >_{\Psi_t} \; : < P >_{\eta_t} = \int \{\hbar\nabla \log \eta_t(q)\}\eta_t^*(q)\eta_t(q)dq = \hbar \int \eta_t^*(q)\nabla\eta_t(q)dq$

<u>NB</u> : <u>or</u>, after integration by parts, $-\int \eta_t(q)\nabla\eta_t^*(q)dq$

$(\hbar\nabla \log \eta_t(q))$ and $(-\hbar\nabla \log \eta^*_t(q))$ represent 2 drifts of <u>same</u> X_t , one w.r.t. increasing $\mathcal{P}_t$, starting from $\rho_s(dq)$, the other decreasing from $\rho_u(dq)$.

Time reversal $=$ Schrödinger's Euclidean version of Complex conjugation in L^2 , associated to product form of $\rho_t(dq)$.

$\exists$ many joint probabilities $m(dx, dz)$ with <u>same</u> given marginals $\rho_s(dx), \rho_u(dz)$. Above $M(dx, dz)$ is only <u>Markovian</u> one, chosen a priori by Schrödinger. Non-Markovian Bernstein processes correspond to <u>mixture</u> of states (Quantum <u>Statistical</u> Physics), not considered here. Only in this context, a notion of <u>Entropy</u> should be justified (Cf. Von Neumann).

Connection with Mass transportation $\longrightarrow$ <u>Joint probability</u> $M(dx, dz)$ $\longrightarrow$ Cf. Christian Léonard.

3) Stochastic geometric dynamics according to L. Schwartz

Second order (SO) tangent vectors $\in \tau_q^s M \supset TM$

$$A = A^i \frac{\partial}{\partial x^i}\Big|_q + A^{jk} \frac{\partial^2}{\partial x^j \partial x^k}\Big|_{q\in M}$$

For $dX(t) = B(X(t), t)dt + \sigma_l^i(X(t))dW^l(t)$

$$(DX)^j = \lim_{\Delta t \downarrow 0} E[\frac{X^j(t+\Delta t) - X^j(t)}{\Delta t}|\mathcal{P}_t]$$

Flat case, $\hbar > 0$ $$= \left(\frac{\partial}{\partial t} + B^i \nabla_i + \frac{\hbar}{2}\Delta\right) X^j = B^j(X(t), t)$$

$$(QX)^{jk} = \lim_{\Delta t \downarrow 0} E[\frac{(X^j(t+\Delta t) - X^j(t))(X^k(t+\Delta t) - X^k(t))}{\Delta t}|\mathcal{P}_t]$$

Def. : (DX, QX) = Process in $T^S M$. (SO tangent bundle)

SO covectors $\in (\tau^*)^s M$:

$$\alpha = \alpha_i \, d^2 x^i \big|_q + \frac{\alpha_{jk}}{2} \, dx^j dx^k \big|_q$$

Duality $< \alpha(q), A >= \alpha_j A^j + \alpha_{jk} A^{jk}$

Fundamental SO forms: $d^2 f$ and $df \cdot dg$ s.t.

$$< d^2 f, A >= Af \quad , \quad < df \cdot dg, A >= A(f \cdot g) - f\, Ag - g\, Af \equiv \Gamma_A(f, g)$$

(Carré du champ)

Restriction to classical cotangent bundle (Phase space) $T^* M$:

$d^2 f\big|_{T^* M} = df$, $df \cdot dg|_{T^* M} = \frac{1}{2}\Big(d(fg) - fdg - gdf\Big) = 0$ (Leibniz & Schwartz)

SO Poincaré form on $(\tau^*)^s M$

$$\omega_{SO} = p_i d^2 x^i + \frac{1}{2} O_{jk} dx^j dx^k$$

Def. $\Omega \equiv -d^2 \omega_{SO}$

with associated “Hamiltonian" H , $\Omega(A_H, B) = d^2 H(B)$, $\forall$ SO vector field B

$\Rightarrow$ General stochastic Hamiltonian equations :

If $\exists$ a (Lévi-Civita) connection ∇ , $\exists$ class of (random) Hamiltonian functions $H_\hbar$ built from classical (Euclidean) $H_0(x,p)$

$$H_\hbar(x,p,o) = H_0(x,p) + \frac{\hbar}{2} g^{ij}(o_{ij} - \Gamma^k_{ij}(x) p_k) \quad \text{s.t.}$$

$$\begin{cases} D_\nabla X = \nabla_p H_0 & \text{for } (D_\nabla X)^i = (DX)^i + \frac{1}{2}\Gamma^i_{jk}(QX)^{jk} \\ & \qquad \underline{\text{true}} \text{ vector !} \\ \frac{\bar{D}}{dt} p = -d_x H_0 & \qquad \frac{\bar{D}}{dt} = \frac{\partial}{\partial t} + \nabla_{D_\nabla X} + \frac{1}{2}\Delta_{LD} \end{cases}$$

On $\underline{M = \mathbb{R}^n}$, for $H_0(x,p) = \frac{1}{2}|p|^2 - V(x)$,

$H_\hbar = H_0 + \frac{\hbar}{2}\mathrm{Tr}O$, $O = \nabla \cdot p$ Probabilistic quantization.

Relation with Schrödinger's problem

Pick $\eta > 0$ solving $\hbar \frac{\partial \eta}{\partial t} = -\frac{\hbar^2}{2}\Delta\eta + V\eta$, $\eta_u > 0$ given, $s \leq t \leq u$. Then

$(DX)^i(t) = \frac{\partial}{\partial x^i} \log \eta(X(t), t)$, $(QX)^{jk}(t) = \hbar\, \delta^{jk}$

(Euclidean) Lagrangian for H_0 , $L_0(x, \dot{x}) = \frac{1}{2}|\dot{x}|^2 + V(x)$

Stochastic E-L :

$$\frac{\bar{D}}{dt}\Big(d_{\dot{x}} L_0(X(t), D_\nabla X(t))\Big) - d_x L_0(X(t), D_\nabla X(t)) = 0$$

A $*$ operation provides $\mathcal{F}_t$ counterparts.

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