Geometry for Quantum Science Group
ITI Quantum Science and Nanomaterials
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Quantisation and Path Integrals

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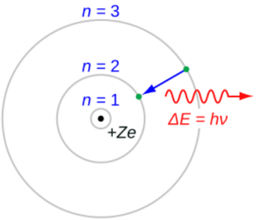
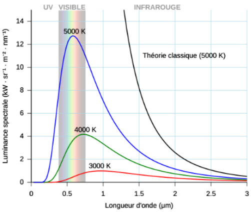
Contents

The dark cloud above classical physics

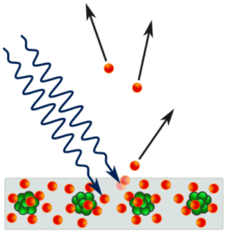
- Atomic spectra
- Black body radiation
- Photoelectric effect



(a) JabberWork, File :Bohr atom model.svg



(b) Darth Kule, File :Black body-fr.svg



(c) Ponor, File :Photoelectric effect in a solid - diagram.svg

$\longrightarrow$ from continuous to discrete observables.

Quantum numbers: adiabatic invariants of quantised systems.

Bohr-Sommerfeld rule

Let q be a periodic coordinate with conjugate momentum p. Then there is a quantum number n such that

$$\oint p \, \mathrm{d}q = nh \tag{1}$$

where h is Planck's constant (the quantum of action).

$\longrightarrow$ from dynamics to statics.

Quantum observables

[picture of phase space]

Observable in classical physics: function on phase space.

Quantum observable: integral of a classical observable / function of phase space curves.

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Quantisation in the Hilbert space

The five postulates:

1. Superposition principle
2. Quantisation principle
3. Born's rule
4. Spontaneous collapse
5. Schrödinger's equation

How do we make sense of 2.?
$\longrightarrow$ connecting classical to quantum observables.

Formally replace in the Hamiltonian all observables by operators.

Since classical observables are functions of (q_k, p_k), quantum observables become functions of $(\hat{q}_k, \hat{p}_k)$ (forgetting about spin).

$\longrightarrow$ just describe the algebra of canonical variable operators:

Heisenberg commutation relations

$$\left[\hat{q}_i, \hat{p}_j\right] = i\hbar\delta_{ij} \tag{2}$$

$$\left[\hat{q}_i, \hat{q}_j\right] = 0 \tag{3}$$

$$\left[\hat{p}_i, \hat{p}_j\right] = 0 \tag{4}$$

$\longrightarrow$ enforces Heisenberg indetermination relations.

More generally:

$$\left[\hat{f}, \hat{g}\right] = i\hbar\widehat{\{f, g\}} \tag{5}$$

But...

Groenewold theorem

There is no map from phase space to the space of operators that simultaneously

1. sends 1 onto $\hat{\mathbb{I}}$;
2. sends q_k onto $q_k\cdot$ and p_k onto $i\hbar\frac{\partial\cdot}{\partial q_k}$;
3. preserves polynomials;
4. satisfies eqn 5.

Beyond Dirac's quantisation

Best we can do: only preserve polynomials up to degree 3.
$\longrightarrow$ **Weyl's transform** (tiens tiens).

Leads to **deformation quantization** when generalized to arbitrary Poisson manifolds.
$\longrightarrow$ Weyl's transform replaced by the Kontsevich quantisation formula.

Physical interpretation becomes awkward
+ Lorentz-covariance not explicit for relativistic theories
+ Heisenberg's indeterminacy: quantum states are not even measurable...

Should we do something *completely different?*

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The sum-over-paths picture

From Bohr-Sommerfeld theory:

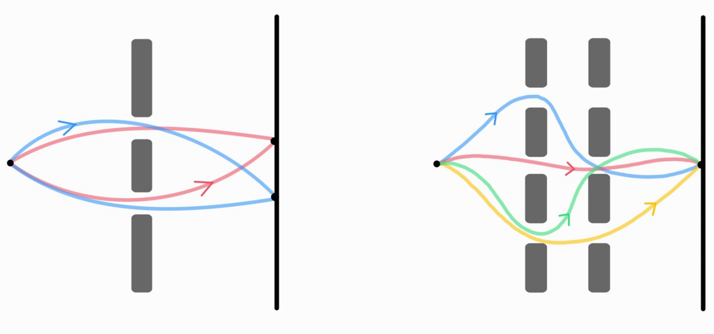
- quantum states are curves in phase space (paths in physical space);
- quantum observables are functions of phase space curves.

From Young's slits experiment:

- a particle passes through both slits since both paths *interfere*;
- this generalizes to an arbitrary number of slits.

From the correspondence principle:

- in the classical limit, there is only one path that counts.



What is the probability to propagate from x_0 to y_1? to y_2?

$$G(x_0, t_0, x_1, t_1) = \langle x_1 | \mathrm{e}^{-i(t_1 - t_0)\hat{H}/\hbar} | x_0 \rangle = \sum_n \langle x_1 | E_n \rangle \, \langle E_n | \mathrm{e}^{-i(t_1 - t_0)\hat{H}/\hbar} | x_0 \rangle \tag{6}$$

$$= \sum_n \psi_n(x_1) \psi_n^*(x_0) \mathrm{e}^{-i(t_1 - t_0)E_n/\hbar} \tag{7}$$

Definition of the path integral

$$G(x_0, t_0, x_1, t_1) = \int_{x(t_0)=x_0}^{x(t_1)=x_1} \mathcal{D}x(t) \mathrm{e}^{iS[x]/\hbar} \tag{8}$$

where we apply the **time-slicing** procedure

$$\mathcal{D}x(t) = \lim_{N\to\infty} \mathrm{e}^{-i\pi/4} \sqrt{\frac{m}{2\pi\hbar\epsilon}} \prod_{n=1}^{N-1} \left[\int \mathrm{d}x_n \, \mathrm{e}^{-i\pi/4} \sqrt{\frac{m}{2\pi\hbar\epsilon}} \right] \tag{9}$$

with $N = (t_1 - t_0)/\epsilon$

$\longrightarrow$ classical limit.

$G(x_0, t_0, x_1, t_1)$ is called the **propagator** of the particle.

Where does it come from?

$$i\hbar \frac{\partial}{\partial t} G = HG \tag{10}$$

$$G(x_0, t_0, x_1, t_0) = \delta(x_1 - x_0) \tag{11}$$

and defining the *retarded propagator* $G_R = G\Theta(t_1 - t_0)$

$$\left(i\hbar \frac{\partial}{\partial t} - H\right) G_R = \delta(x_1 - x_0)\delta(t_1 - t_0) \tag{12}$$

$$G_R(x_0, t_0, x_1, t_0) = \delta(x_1 - x_0) \tag{13}$$

$\longrightarrow$ G_R is the **Green function** associated to Schrödinger's equation.

Green functions for PDEs

Let D be a linear differential operator. Solve for ϕ the partial differential equation

$$D\phi(x) = j(x). \tag{14}$$

A **Green function** for D is any solution of

$$DG(x_0, x) = \delta(x - x_0). \tag{15}$$

Green functions theorem

Let G be a Green function for D. Then

$$\phi(x) = \int G(x_0, x) j(x_0) \, \mathrm{d}x_0 \tag{16}$$

is a solution of eqn 14.

Nonrelativistic quantum mechanics = 1D field theory

Generalization to arbitrary quantum field theories

$$G(\varphi, \mathcal{N}) = \int\limits_{\phi|_{\partial\mathcal{N}}=\varphi} \mathcal{D}\phi(x) e^{iS[\phi]/\hbar} \tag{17}$$

with $\mathcal{N}$ an arbitrary spacetime domain with φ a field on $\partial\mathcal{N}$.

$\longrightarrow$ explicit Lorentz-covariance.

However, quantization and unitarity are not explicit anymore.

Quantum-statistical path integral

Time $\longrightarrow$ Temperature.

Partition function

$$Z(\beta) = \mathrm{Tr}\, \mathrm{e}^{-\beta \hat{H}} = \int \mathrm{d}x \, \langle x | \mathrm{e}^{-\beta \hat{H}} | x \rangle = \oint_{t_1 - t_0 = -i\hbar\beta} \mathcal{D}x(t) \mathrm{e}^{iS[x]/\hbar} \tag{18}$$

then

$$\left\langle \hat{O} \right\rangle_\beta = \frac{1}{Z(\beta)} \int \mathrm{d}x \, \langle x | \mathrm{e}^{-\beta \hat{H}} \hat{O} | x \rangle = \frac{1}{Z(\beta)} \int_{t_1 - t_0 = -i\hbar\beta} \mathrm{d}x \, \mathrm{d}y \, G(y, t_0, x, t_1) \, \langle y | \hat{O} | x \rangle \, . \tag{19}$$

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Large time limit and expectation values

$$G(x_0, t_0, x_1, t_1) = \sum_n \psi_n(x_1)\psi_n^*(x_0)\mathrm{e}^{-i(t_1-t_0)\hat{E}_n/\hbar}. \tag{20}$$

Setting $E_0 = 0$ and taking $t_1 \to -i\infty$ and $t_0 \to +i\infty$ yields

$$G_\infty = \psi_0(x_1)\psi_0^*(x_0) = \langle x_1|E_0\rangle \langle E_0|x_0\rangle \tag{21}$$

$\longrightarrow$ probability amplitude for a particle in the ground state to be at x_0 and x_1
$\longrightarrow$ *field* point of view.

$$\langle 0|\hat{O}|0\rangle = \int_{\mathcal{M}} \mathcal{D}\phi O[\phi]\mathrm{e}^{iS[\phi]/\hbar} \tag{22}$$

on the whole manifols $\mathcal{M}$ $\longrightarrow$ time-ordered product.

Chapman-Kolmogorov equation

$$G(x_0, t_0, x_1, t_1) = \int \mathrm{d}x \, G(x_0, t_0, x, t) G(x, t, x_1, t_1) \tag{23}$$

Sewing law

$$\int\limits_{\Sigma_1 \to \Sigma_2} \mathcal{D}\phi \mathrm{e}^{iS[\phi]/\hbar} = \int_{\Sigma'} \mathcal{D}\varphi' \int\limits_{\Sigma_1 \to \Sigma_2}^{\phi|_{\Sigma'} = \varphi'} \mathcal{D}\phi \mathrm{e}^{iS[\phi]/\hbar}. \tag{24}$$

Fermionic integrals

Equal time canonical anticommutation relations

$$\left\{\psi_\alpha(x), \psi_\beta^\dagger(y)\right\} = \delta^{\alpha\beta}\delta^{(3)}(x-y) \tag{25}$$

Grassmann variables: Grassman algebra of anticommuting generators $\{\theta_1, \theta_2\}$

$$\theta_1\theta_2 = -\theta_2\theta_1 \tag{26}$$

$\longrightarrow$ each $\psi(x)$ and $\psi^\dagger(x)$ for each spacetime point are Grassmann variables.

Problems of the path integral

Nonrelativistic path integral is defined through **Wiener measure**

$\longrightarrow$ connection with Schrödinger's equation ensured by the Feynman-Kac formula.

However

Ill defined in general...
$\longrightarrow$ perturbative quantum field theory
$\longrightarrow$ functorial field theory.

Acknowledgements

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