Visualising Quantum Mechanics

based on Bernd Thaller: Visual Quantum Mechanics

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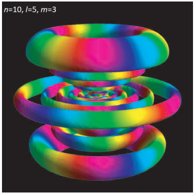

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Outline

- Classical Newtonian Mechanics in Hamilton Formalism
- Axioms of Quantum Mechanics
- Visualising Complex function
- Fourier Transformation
- Time Evolution
- Interaction-free Measurement

Two semesters of Newtonian mechanics in two slides

1/2

- classical particles lives in phase space $(p, q) \in \mathbb{R}^d \times \mathbb{R}^d$
- each system described by its Hamiltonian

$$H(p, q, t) = \sum_{j=1}^{N} p_j \dot{q}^j - L(q, \dot{q}, t)$$

- motion described by equations of motion

$$\dot{q}^j = \frac{\mathrm{d}H}{\mathrm{d}p_j}, \quad \dot{p}_j = -\frac{\mathrm{d}H}{\mathrm{d}q^j}$$

- time evolution of a function f described by

$$\frac{\mathrm{d}f}{\mathrm{d}t} = \frac{\partial f}{\partial t} + \{f, H\}$$

where

$$\{f, g\} = \sum_{j=1}^{N} \left(\frac{\partial f}{\partial q^j} \frac{\partial g}{\partial p_j} - \frac{\partial f}{\partial p_j} \frac{\partial g}{\partial q^j} \right)$$

is a Poisson bracket in canonical coordinates

2/2

1D harmonic oscillator

- Hamiltonian

$$H = \frac{p^2}{2m} + \frac{k}{2}q^2$$

where $k = m\omega^2$

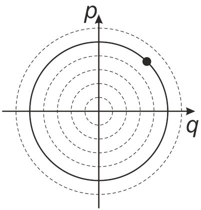
- equations of motion

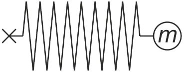
$$\dot{q} = \frac{p}{m}, \quad \dot{p} = -kq$$

- solution

$$\ddot{q} = -\frac{k}{m}q, \quad \dot{p} = -kq$$

$$q = -A\cos\left(\sqrt{\frac{k}{m}}t + B\right), \quad \dot{p} = A\sqrt{km}\sin\left(\sqrt{\frac{k}{m}}t + B\right)$$





Let's go quantum

States: Axiom 1a,b,c

Definition of the playground

State space-Q1a

The state space of a quantum mechanical system has the structure of a complex separable Hilbert space H.

State-Q1b

A ray, i.e., a one–dimensional subspace in H corresponds to any state of the system under consideration.

Observable-Q1c

A self–adjoint operator on the state space is associated with any observable of the system.

States: Axiom 1a,b,c

Definition of the playground

State space-Q1a

The state space of a quantum mechanical system has the structure of a complex separable Hilbert space H.

Generalization-Q1b'

A statistical operator (density matrix) on the state space is associated with any state of the system.

Observable-Q1c

A self–adjoint operator on the state space is associated with any observable of the system.

Measurement: Axiom Q2a,b

Generalization-Q2a

The possible outcome of measuring the observable A will be the points of the spectrum $\sigma(A)$ of the operator A.

Generalization-Q2b

The probability of finding the measured value in a Borel set $\Delta \subseteq \mathbb{R}$ is

$$w(\Delta, A; \psi) = \int_\Delta d(\psi, E_\lambda^{(A)}\psi) = \|E_A(\Delta)\psi\|^2 .$$

Q2b implies that the mean value of measurement is given by

$$\langle A \rangle_\psi = (\psi, A\psi) .$$

Measurement: Axiom Q2a,b

Generalization-Q2a

The possible outcome of measuring the observable A will be the points of the spectrum $\sigma(A)$ of the operator A.

Generalization-Q2b'

The probability that measuring an observable A on the system in a state W we find a value contained in a Borel set $\Delta \subseteq \mathbb{R}$ is

$$w(\Delta, A; W) = \mathrm{Tr}(E_A(\Delta)W)\,.$$

The mean value of measurement is given by

$$\langle A\rangle_W := \int_{\mathbb{R}} \lambda \mathrm{d}\mathrm{Tr}(E_\lambda^{(A)} W) = \mathrm{Tr}(AW) = \mathrm{Tr}(\overline{WA})\,.$$

provided that right side makes sense.

Measurement: Axiom Q3

Measurement-Q3

If the result of the experiment is positive (the measured value is contained in the set Δ), the system after the measurement will be in the state described by the unit vector

$$\frac{E_A(\Delta)\psi}{\|E_A(\Delta)\psi\|}$$

in the opposite case we have to replace

$$\frac{E_A(\mathbb{R}\setminus\Delta)\psi}{\|E_A(\mathbb{R}\setminus\Delta)\psi\|}\,.$$

Measurement-Q3'

Suppose that the system before measurement is in a state W. If the result is positive (the measured value is contained in the set Δ), then the state after measurement is described by the statistical operator

$$W := \frac{E_A(\Delta)WE_A(\Delta)}{\mathrm{Tr}(E_A(\Delta)W)}\,.$$

Time evolution-Q4

Time evolution-Q4

- The time evolution of any state of the system is described by a unitary propagator, $W_t = U(t,s)W_sU(t,s)^{-1}$ or $\psi(t) = U(t,s)\psi(s)$ where $s,t \in J$ is from the interval where the system is undisturbed.
- The propagator of a conservative system with the Hamiltonian H is given by $U(t) = e^{-iHt}$ for any $t \in \mathbb{R}$.

Schrödinger equation

If $W_sD(H) \subset D(H)$ is valid at some instant s, then the function $t \to W_t\phi$ is differentiable for any $\phi \in D(H)$ and obeys the equation

$$i\frac{\mathrm{d}}{\mathrm{d}t}W_t\phi = [H, W_t]\phi\,.$$

In particular, if $\psi_s \in D(H)$ for some s, then $t \to \psi_t$ is differentiable and

$$i\frac{\mathrm{d}}{\mathrm{d}t}\psi_t = H\psi_t\,.$$

Complex function in graphs

- we need to work with complex functions
- we need to represent two components
- how to repsesent phase and modulus

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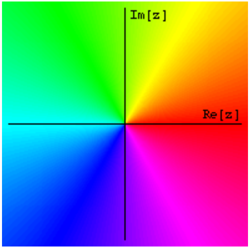


Figure: Complex phase representation

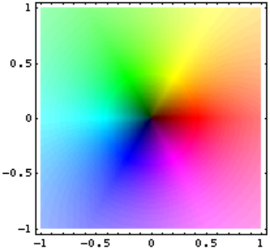


Figure: Modulus tranformed to brightness

Fourier transform

- Fourier transform is defined as

$$\hat{\psi}(k) = (\mathcal{F}\psi)(k) = \frac{1}{(2\pi)^{n/2}} \int_{\mathbb{R}^n} e^{-ik\cdot x}\psi(x)\mathrm{d}^n x$$

- Transform multiplication by a variable to derivative and vice versa
- Translation in position space corresponds to a phase shift in momentum space and vice versa
- In Quantum mechanics we can not measure non-commuting variables at once

$$\Delta_\psi A \Delta_\psi B \geq \frac{1}{2}|(\psi, [A, B]\psi)|$$

  - Uncertatinty principle
- Using Fourier transform we can generalize the notion of the derivative to non-integer orders

$$f\left(\frac{d}{dx}\right)\psi = \mathcal{F}^{-1} f(ik)\hat{\psi}$$

  - Generalized derivative

Commutation

- Commutation of two rotations
  One can check
  $$R_x(\phi)R_y(\phi) \simeq R_z(\phi^2)R_y(\phi)R_x(\phi)$$
  which holds up to ϕ^3 where $R_j(\phi) = \exp(-iL_j\phi)$
  - Rotations does not commute
- Commutation of shift in position and momentum
  Weyl relation: The unitary groups τ_a (translations in position space) and μ_b (translations in momentum space) satisfy the relations
  $$e^{-iab}e^{-ipa}e^{-ixb} = \tau_a\mu_b = e^{-iab}\mu_b\tau_a = e^{-iab}e^{-ixb}e^{-ipa}$$
  for all $a, b \in \mathbb{R}$
  - Shift in x and in p does not commute
  - Shift in x and in p does not commute

Gaussian packets

- Time evolution govern by Schrödinger equation

$$i\frac{\mathrm{d}}{\mathrm{d}t}\psi_t = H\psi_t\,.$$

- Evolution of a free particle can be written as

$$\psi(x,t) = \frac{1}{(2\pi)^{n/2}}\int_{\mathbb{R}^n} e^{ik\cdot x - ik^2 t/2}\hat{\psi}_0(k)\mathrm{d}^n k$$

- Time evolution of an eigenstate $\psi(t) = e^{-iEt}\psi(0)$
- There is symmetry of time evolution with respect to time reversal. The wave packet at time $-t$ is complex conjugate of the wave packet at time t
  - Free particle at rest
  - Free particle with average momentum 2

Bounded domains

- Potential well
  - Dirichlet well eigenstates in a box
  - Neumann well eigenstates in a box
- Self-interference of a Gaussian packet on a circle
  - Self-interaction of Gaussian packet on a circle with Schrödinder cat states
  - Self-interaction of Gaussian packet on a line with periodic boundary conditions

Domain matters

- Dirichlet Laplacian on interval $(0, 1)$
- Every state of a particle in a Dirichlet box depends periodically on time with period $T = 4/\pi$
- If $\psi(x, 0) = 1$, then $\psi(x, t)$ is a step function at every time t for which t/T is a rational number.
- If $\psi(x, 0) = 1$, then $\psi(x, t)$ is not differentible in t nor x.
  - Putting initial condition outside of operator domain

Coulomb states

- Coulomb states in $\mathbb{R}^2$
- Eigenstates just change phase and not modulus
- Superpositions have more complicated behaviour
- Linear combination of state with different energy and quantum number leads to rotation
  - The state $|8,3\rangle$
  - The state $|8,3\rangle + |8,-3\rangle$
  - The state $|6,1\rangle + |6,-2\rangle + |6,4\rangle$
  - The state $|5,3\rangle + |6,3\rangle$
  - The rotating state $|4,-1\rangle + |7,4\rangle$
  - The rotating state $|6,-2\rangle + |7,3\rangle$

Free-fall

- Behaviour of the system $H = -\frac{1}{2m}\Delta - \lambda z$
  - Free-fall
  - Vertical throw
  - Parabolic trajectory
  - Quasiclassical motion
  - Bouncing ball in the box

Movement through Stern-Gerlach device

- Movement of the spin particle in inhomogenneous magnetic field
- Pauli operator

$$H_{\text{pauli}} = \frac{1}{2m_e}(p + eA(x))^2 - \frac{e\hbar}{2m_e}\begin{pmatrix} B_3(x) & B_1(x) - iB_2(x) \\ B_1(x) + iB_2(x) & -B_3(x) \end{pmatrix}$$

where $B = \nabla \times A$

- Standard Stern-Gerlach device
- Filter of spin down
- Filter of spin up

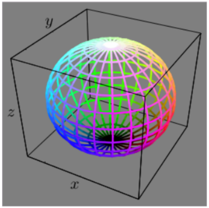
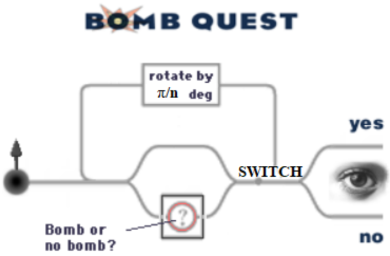


Figure: Visualization of the local spin-direction

Bomb testing

- Malicious person gives you a black box with something in it
- Claim is that there is a bomb which explodes after interaction with a single photon
- We can check the existence of the bomb without touching it
- Rotating spin by π/n leads to probability of the missing the bomb $\cos^2(\pi/n)$
- Total probability of successful check $\cos^{2n}(\pi/n)$
- Experimentally done Anton Zeilinger et.al.



References

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- *Thaller, Bernd* Advanced visual quantum mechanics. Springer Science & Business Media, 2005.

Thank you for your attention