Advanced Graduate Quantum Mechanics

summer term 2024-25

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Tutorials: **Krystian jabłonowski**

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Rules

- Lectures are on Tuesdays at 14:15-16:00 in B0.21 room.
- Tutorials are on Wednesday at 10:15-12:00 in B0.21 room.
- Home problems will be offered but not be checked. Some of these problems or similar ones might occur during a colloquium or an exam.
- Standard way of passing the course
  - Mid term written exam (Kolokwium), max 50 pts.
  - Final written exam, max 50 pts.
  - Oral exam (in uncertain cases)
- Second (resit) exam to pass the course
  - Written exam, max 100 pts.
  - Oral exam (in uncertain cases)

  Final grade is based on total score points normalized to 100 and determined as follows:

  5+ for 99-100 pt.
  5 for 90-98 pt.
  4+ for 81-89 pt.
  4 for 72-80 pt.
  3+ for 62-71 pt.
  3 for 50-61 pt.
  2 for 0-49 pt.

  Warning: points from the mod term exam and final exam and from the second exams do not sum up.

Dates of exams:

colloquium, April 16th, 2025, 11:00-13:00, room B0.21

written exam I, June 17th, 2024, 9:00-13:00, room ???

oral exam I, on e-mail note

written exam II, September ?th, 2025, 9:00-13:00, room ???

oral exam II, on e-mail note

1 Week I

1.1 Lecture

I - Symmetries in Quantum Mechanics

&1. *Axioms of quantum mechanics* - Postulates of quantum mechanics, pure and mixed states, measurement on pure and mixed states, ...

1.2 Tutorial

1. *Conservation of momentum in classical physics* - Consider a single particle moving in a homogeneous space. Within the Lagrangian formalism show that the momentum of the particle is conserved in time.

2. *Conservation of energy in classical physics* - Consider a single particle moving in space in a time independent potential. Within the Lagrangian formalism show that the energy of the particle is conserved in time.

3. *Conservation of angular momentum in classical physics* - Consider a particle moving in an isotropic space. Within the Lagrangian formalism show that the angular momentum of the particle is conserved in time.

4. *Conserved quantity for a charge classical particle in a homogeneous electric field* - Derive a conservation law and find a conserved quantity for a classical particle with charge q and mass m moving in a homogeneous electric field with an intensity $\mathbf{E}$.

5. *Ehrenfest theorem* - Prove the Ehrenfest theorem.

1.3 Homework problems

1. *Conserved quantity for a charge classical particle in a homogeneous magnetic field* - Derive a conservation law and find a conserved quantity for a classical particle with charge q and mass m moving in a homogeneous magnetic field with an induction $\mathbf{B}$.

2. *Angular momenta in different reference frames* - (a) What is the connection between the angular momenta in two reference systems which are at rest relative to each other and whose origins are separated by the distance vector $\mathbf{a}$?
(b) What is the relation between the angular momenta in two inertial reference systems which move with velocity $\mathbf{V}$ relative to each other?

3. *Runge-Lenz-Laplace vector in the Kepler-Coulomb problem* - Consider a single particle moving in a central force $\mathbf{F}(\mathbf{r}) = -\alpha\mathbf{r}/r^3$. Introduce a vector $\mathbf{J} = \mathbf{p}\times\mathbf{L} - \beta\mathbf{r}/r$, where $\mathbf{p}$ and $\mathbf{L}$ are momentum and angular momentum, respectively. Check that $\mathbf{J}\cdot\mathbf{L} = 0$ and $J^2 = 2HL^2 + \beta^2$, where $H = \mathbf{p}^2/2 - \beta/r$ is the energy (Hamiltonian) per mass m, and $\beta = \alpha/m$. Prove that

$$\frac{d}{dt}\left(\dot{\mathbf{r}}\times\mathbf{L} - \alpha\frac{\mathbf{r}}{r}\right) = 0,$$

so $\mathbf{J}$ is invariant in time. How many components of $\mathbf{J}$ are in fact independent? Conclude why $\mathbf{J}$ and $\mathbf{r}$ are in the plane perpendicular to $\mathbf{L}$ and how the motion of a particle is constrained. In the polar coordinate system parametrize $\mathbf{J}$ and $\mathbf{r}$ and write $\mathbf{J}\cdot\mathbf{r} = Jr\cos(\phi-\phi_0)$, where ϕ and ϕ_0 are angles between horizontal axis and the vectors $\mathbf{r}$ and $\mathbf{J}$, respectively. Derive that the shape of the particle's trajectory is expressed by

$$r(\phi) = \frac{p}{1+e\cos(\phi-\phi_0)},$$

where $p = L^2/m\alpha$ and $e = J/\alpha = \sqrt{1+2EL^2/m\alpha^2}$. What are interpretations of these parameters? Think about the role of the vector $\mathbf{J}$ in this solution.

2 Week II

2.1 Lecture

... Ehrenfest theorem, conservation laws.

&2. *Symmetry transformations* - definition of a symmetry transformation in quantum mechanics, Wigner's theorem, conservation laws obtained from a symmetry, linear and antilinear operators, infinitesimal symmetry transformations, symmetry generators as observables, symmetry and degeneracy, classification of different symmetry transformations: continuous (space translations, time translations, rotations) and discrete (periodic translation in space, periodic translation in time, parity, time reversal).

2.2 Tutorial

1. *Units of bra and ket vectors* - What are units of bra and ket vectors in quantum mechanics. Discussion based on: *Do bras and kets have dimensions?*, C. Semay and C.T. Willemyns, Eur. J. Phys. **42**, 025404 (2021) (arXiv:2008.03187).

2. *Equation of symmetry generator* Assuming that $\hat{\Omega}(t)$ is a generator of the symmetry $\hat{U}(t) = \exp(-ia\hat{\Omega}(t))$ and $\hat{H}$ is the Hamiltonian of the system derive an equation satisfied by $\hat{\Omega}$.

3. *Derivation of Pauli equation* - Consider an invariant Hamiltonian

$$\hat{H} = \frac{(\vec{\sigma}\cdot\hat{\mathbf{p}})^2}{2m},$$

where $\vec{\sigma}$ is a three component vector made of 2×2 matrices. Show that if these matrices obey an algebra of Pauli matrices

$$\sigma_i\sigma_j + \sigma_j\sigma_i = 2\delta_{ij},$$

$$[\sigma_i, \sigma_j] = 2i\epsilon_{ijk}\sigma_k,$$

then the Hamiltonian is equivalent to the one for free particles. For this you need to show

$$(\vec{\sigma}\cdot\mathbf{a})(\vec{\sigma}\cdot\mathbf{b}) = \mathbf{a}\cdot\mathbf{b} + i\vec{\sigma}\cdot(\mathbf{a}\times\mathbf{b}).$$

Next, introducing a magnetic field via the vector potential and the minimal coupling procedure $\hat{\mathbf{p}}\to\hat{\mathbf{p}} - q\mathbf{A}$ derive the Pauli Hamiltonian for a spin 1/2 particles in an external magnetic field $\mathbf{B}$. This problem follows an article in Am. J. Phys. **49**, 645 (1981).

2.3 Homework problems

1.

3 Week III

3.1 Lecture

&3. *Continuous symmetry transformations* - active and passive view on space and time transformations, <u>translation in space</u>, infinitesimal translation and its generator, symmetry operator of arbitrary translation, homogeneity of space and conservation of momentum, <u>translation in time</u>, infinitesimal translation and its generator, symmetry operator of arbitrary translation, homogeneity of time and conservation of energy, <u>rotation in space</u>, infinitesimal rotation and its generator, symmetry operator of arbitrary rotation, isotropy of space and conservation of angular momentum.

3.2 Tutorial

1. *Conservation law in a uniform external electric field* - Derive a quantum mechanical generator for the translational symmetry of a charged particle in a homogeneous electric field with the intensity $\mathbf{E}$.

2. *Mixed state measurement* - Derive the result, probability, and the state after the measurement of the energy on a mixed state

$$\hat{\rho} = \sum_i q_i|\psi_i\rangle\langle\psi_i|,$$

where

$$|\psi_i\rangle = \sum_n \sqrt{p_n} E^{i\alpha_n} |E_n\rangle$$

is a superposition of the eigen energy states.

3.3 Homework problems

1. *Algebraic relations for translation operators* - Show that

$$\left(\frac{i}{\hbar}\hat{p}\right)^n \hat{B}(x) = \sum_{\nu=0}^{n} \left(\begin{array}{c} n \\ \nu \end{array}\right) \frac{\partial^\nu \hat{B}}{\partial x^\nu} \left(\frac{i}{\hbar}\hat{p}\right)^{n-\nu},$$

where $\hat{p}$ is a momentum operator and $\hat{B}(x)$ is every differentiable operator. Next, using the result above, calculate $\hat{U}(a)^\dagger \hat{A}(x) \hat{U}(a)$ where $\hat{U}(a) = e^{-ia\hat{p}/\hbar}$.

2. *Conservation law in a uniform external magnetic field* - Derive a quantum mechanical generator for the translational symmetry of a charged particle in a homogeneous magnetic field with the induction **B**.

4 Week IV

4.1 Lecture

&4 *Discrete symmetry transformations* - Discrete translational symmetry in space, periodic potential and primitive translational vectors of a crystal structure (lattice), Bloch theorem and simultaneous eignestates of symmetry operator of discrete translations and a periodic Hamiltonian, Bloch wave function, quasimomentum in crystals, Discrete translations in time, time dependent periodic Hamiltonian, properties of the evolution operators for periodic Hamiltonians, Floquet Hamiltonian, Floquet theorem, Floquet eigenstates in time periodic systems, ...

4.2 Tutorial

1. *Rotation of spin one particle wave function* - Find a transformation operator for a three-component vector wave function (field). Conclude that it describes a spin one particle.

2. *Periodic lattices, Brillouin zones, Bloch's theorem, part I* - Consider one dimensional problem with a periodic potential $V(x) = V(x \pm na)$, $n \in Z$. By imposing a periodic boundary condition ina finite system with N lattice sites find eigenvalues of the discrete translation operator $\hat{U}(a)$, which $\hat{U}(a)|n\rangle = |x + a\rangle$. Discuss number of those eigenvalues and a periodicity of the solution in a reciprocal space. Identify the first Brillouin zone and a periodic vector in reciprocal space.

3. *Lattice (discrete) Fourier transform* - Define the Lattice (discrete) Fourier transform for a periodic sequence $A_{j+N} = A_j$, i.e.,

$$A_j = \frac{1}{\sqrt{N}} \sum_k a_k e^{ikaj},$$

with $k = 2\pi m/aN$ and $-N/2 < m \leqslant N/2$, and prove the lattice sum

$$\frac{1}{N} \sum_k e^{ika(j-l)} = \delta_{jl}.$$

Similarly it holds that

$$\frac{1}{N} \sum_j e^{i(k-k')aj} = \delta_{kk'}.$$

4. *Periodic lattices, Brillouin zones, Bloch's theorem, part II* - Construct an eigenkets of $\hat{U}(a)$ and the corresponding eigenfunctions $\Phi_k(x)$. Discuss the Bloch's theorem.

5. *Tight binding model* - Consider an infinite one-dimensional system with a periodic potential $V(x \pm a) = V(x)$. Let $|n\rangle$ be a ground state vector describing a particle localized in the n-th cell of the crystal. The ground state energy is E_0. Assume that,

$$\langle n|m\rangle = \delta_{nm},$$
$$\langle n|\hat{H}|n\rangle = E_0,$$
$$\langle n|\hat{H}|n \pm 1\rangle = -\Delta \leqslant 0,$$

and other amplitudes vanish. Write down the Hamiltonian in $|n\rangle$ base. Find the dispersion relation, energy eigenvalues of particles.

4.3 Homework problems

1. *Rotation of spin one-half particle wave function* - Find how the two-component spinor wave function is transformed under rotations. Show that such a wave function describes a spin one-half particle. Hint: to find the transformation rules for the bispinor wave function you need to discuss an invariance of the probability density and the Pauli equation, cf. W. Greiner's book.

2. *Chain molecule - Tight binding model* - Consider a chain molecule of N atoms. Find the eigenstates and eigenenergies of such a system. Assume a natural boundary condition. Discuss the transition from a single atom $N = 1$ via $N = 2$ and 3 cases to an infinite system and appearance of the continuum band. Hints: Take a one-particle localized base $\{|j\rangle\}$ and expand any state

$$|\psi\rangle = \sum_{j=1}^{N} c_j |j\rangle\ .$$

Solve the Schroedinger equation

$$\hat{H}|\psi\rangle = E|\psi\rangle,$$

assuming that $\langle j|\hat{H}|j\rangle = \alpha$ and $\langle j|\hat{H}|k\rangle = \beta$ for j and k nearest neighbors, and zero otherwise. Prove that $E_m = \alpha + 2\beta\cos(m\pi/(N+1))$ and $c_j^m = \sqrt{2/(N+1)}\sin(mj\pi/(N+1))$. In the case of the natural boundary condition $c_0 = c_{N+1} = 0$, the wave function out of the chain vanishes, being still finite at edges in principle.

3. *Ring molecule - Tight binding model* - Consider a ring molecule of N atoms. Find the eigenstates and eigenenergies of such a system. Assume a periodic boundary condition. Discuss the transition from few atoms to the thermodynamic limit. Discuss the Bloch theorem in the finite and in the infinite systems. Hints: Take a one-particle localized base $\{|j\rangle\}$ and expand any state

$$|\psi\rangle = \sum_{j=1}^{N} c_j|j\rangle \ .$$

Solve the Schrodinger equation

$$\hat{H}|\psi\rangle = E|\psi\rangle,$$

assuming that $\langle j|\hat{H}|j\rangle = \alpha$ and $\langle j|\hat{H}|k\rangle = \beta$ for j and k nearest neighbors, and zero otherwise. Impose the periodic boundary conditions and show that $E_m = \alpha + 2\beta\cos(2\pi m/N)$ and $c_j^m = \exp(i2\pi jm/N)/\sqrt{N}$.

5 Week V

5.1 Lecture

Parity transformation, parity transformation in classical physics, polar and axial vectors and examples, role of parity transformation in quantum mechanics, transformation of different operators under the parity, conservation of parity for parity symmetric Hamiltonians, classification of energy eigenstates under their parity symmetry, even and odd states, Time reversal transformation, reversal of time in classical physics, Newton law, transformation of position, velocity, momentum, force, Maxwell equations, transformation of current, electric intensity, magnetic induction, to be continued, problem with a unitary time reversal operator in quantum mechanics, antiunitary time reversal operator, classification of operators regarding time reversal operation, transformation of a scalar wave function under reversing a time, transformation of spin under time reversing, Kramers degeneracy.

5.2 Tutorial

1. *A quantum particle with a time dependent potential* - Find the exact solution for a problem of a one-dimensional quantum particle described by the following Schrödinger equation

$$i\hbar\frac{\partial\Psi(x,t)}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\Psi(x,t)}{\partial^2 x} - V(t)\Psi(x,t),$$

where $V(t)$ is a time dependent potential, constant in space. Find a solution for time-periodic potential $V(t) = V_0\sin(\Omega t+\theta)$. Check the validity of the Floquet theorem.

2. *Harmonic oscillator with driven time-dependent force* - Find the exact solution of the problem with one-dimensional quantum harmonic oscillator in the presence of a driving force and described by the following Schrödinger equation

$$i\hbar\frac{\partial\Psi(x,t)}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\Psi(x,t)}{\partial^2 x} + \frac{1}{2}m\omega^2x^2\Psi(x,t)$$
$$-xF(t)\Psi(x,t),$$

where $F(t)$ is a time dependent force. Next, discuss an explicit solution for a periodic driving force $F(t) = A\sin(\Omega t)$ and check the validity of the Floquet theorem. Based on P. Hängi, *Quantum transport and dissipation*, chapt. 5.

5.3 Homework problems

1. *A quantum particle in a gravity field with a time dependent force* - Find the exact solution for a problem of a one-dimensional quantum particle in a gravity field described by the following Schrödinger equation

$$i\hbar\frac{\partial\Psi(x,t)}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\Psi(x,t)}{\partial^2 x} + mgx\Psi(x,t)$$
$$-xF(t)\Psi(x,t),$$

where $F(t)$ is a time dependent force, constant in space, and $x \geqslant 0$. Find a solution for time-periodic force $F(t) = A\sin(\Omega t)$. Check the validity of the Floquet theorem. Based on arXiv:2202.01213.

6 Literature

- W. Greiner, B. Müller *Quantum mechanics - symmetries.*
- L.E. Ballentine, *Quantum mechanics. A modern development.*
- A. Messiah, *Quantum mechanics*, vol. I and II.
- J.J. Sakurai, J. Napolitano, *Modern quantum mechanics.*
- L. I. Schiff, *Quantum mechanics.*
- A. Altland, `http://www.thp.uni-koeln.de/Documents/altland_advqm_2012.pdf`
- More to be added in the course.