Advanced Graduate Quantum Mechanics

summer term 2023-24

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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, May 15th, 2024, 11:00-13:00, room B0.21

written exam I, June 19th, 2024, 9:00-13:00, room ???

oral exam I, on e-mail note

written exam II, September 2th, 2024, 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, Ehrenfest theorem, conservation laws.

&2. *Symmetry transformations* - definition of a symmetry transformation in quantum mechanics, Wigner's theorem, conservation laws obtained from a symmetry, ...

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

... 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).

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

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. *Translational symmetry operator* - Construct the unitary translation operator $\hat{U}(\mathbf{a}) = e^{-i\mathbf{a}\cdot\hat{\mathbf{p}}/\hbar}$ for an arbitrary translation vector $\mathbf{a}$.

3. *Translational symmetry operator* - Let $\hat{U}(\mathbf{a})$ is a translation operator and $\hat{O}(\mathbf{a})$ is an observable operator. Show that $\hat{U}(\mathbf{a})^\dagger\hat{O}(\mathbf{a})\hat{U}(\mathbf{a}') = \hat{O}(\mathbf{a}+\mathbf{a}')$, using that $\hat{U}(\mathbf{a})\psi(\mathbf{r}) = \psi(\mathbf{r}-\mathbf{a})$ and $\hat{U}(\mathbf{a})^\dagger\psi(\mathbf{r}) = \psi(\mathbf{r}+\mathbf{a})$, where $\psi(\mathbf{r})$ is a wave function.

4. Two particles of mas m_1 and m_2 in one dimension are interacting with each other with the potential $V(|x_1 - x_2|)$ and the Hamiltonian of this system is

$$\hat{H} = \frac{\hat{p}_1^2}{2m_1} + \frac{\hat{p}_2^2}{2m_2} + V(|x_1 - x_2|).$$

Translation operator acting on the wave function gives

$$\hat{U}(a)\psi(x_1, x_2) = \psi(x_1 - a, x_2 - a).$$

a) Show that

$$\hat{U}(a) = e^{-\frac{i}{\hbar}a\hat{P}},$$

where $\hat{P} = \hat{p}_1 + \hat{p}_2$ is a total momentum.
b) Show that the total momentum is conserved.

2.3 Homework problems

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

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

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 $\hat{U}(a) = e^{-ia\hat{p}/\hbar}$.

3 Week III

3.1 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, ...

3.2 Tutorial

1. *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 $\hat{\Omega}$.

2. *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 $\mathbf{E}$.

3. *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 $\mathbf{B}$.

4. *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).

5. *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.

3.3 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.

4 Week IV

4.1 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.

4.2 Tutorial

1. *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.

2. *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

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

3. *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.

4. *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. *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.

2. *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

II - Spontaneous Symmetry Breaking in Quantum Mechanics

&1. *Methaphysic* - Theory of almost everything (around us), symmetries of general many-body non-relativistic quantum Hamiltonian, existence of phases without a symmetry of their Hamiltonians, some examples, thermodynamic limit, emergency principle.

&2. *Spontaneous symmetry breaking* - Definition of spontaneous symmetry breaking and a Bogoliubov method of its detection, concept of an order parameter, singular (non-commuting) limits in perturbation and number of particles, mathematical and mechanical examples of singular limiting procedure. For more reading: SciPost Phys. Lect. Notes **11**, (2019).

&3. *Spontaneous symmetry breaking in quantum mechanical model - harmonic crystal* - Model of a harmonic crystal in one-dimension, creation and annihilation operator, diagonalization of the Hamiltonian via Fourier transform and Bogoliubov transform, analysis of the excitation spectrum, emergence of new quasiparticles - phonons - Goldstone modes, separate treatment of the zero momentum part of the Hamiltonian, total momentum of the system, existence of *thin spectrum*, its role in thermodynamics and in translationally symmetry breaking in the thermodynamic limit, adding a small translationally symmetry breaking perturbation, non-commutative limits. Based on: Am. J. Phys. **75**, 636 (2007).

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

6.1 Lecture

&4. *Ferromagnet - a prominent exception* - The Heisenberg model, rotational symmetry of the Heisenberg model, exact ferromagnetic ground state without rotational symmetry, definition of orientation vector and its classical behavior in the thermodynamic limit, orthogonality of different oriented ferromagnetic states in the thermodynamic limit, symmetry breaking and classical behavior, low energy excitations of ferromagnets, quadratic dispersion of magnons, spin-waves. [1]

III. Galilean and gauge transformations in quantum mechanics

&1. *Landé-Lévy-Lebonds pseudoparadox* - Discussion of de Broghlie $p = h/\lambda$ and Einstein $E = h\nu$ hypothesis in laboratory and moving frames, Galilean transformation in classical wave physics and classical Doppler effect, based on: Am. J. Phys. **44**, 1130 (1974).

&2. *Galilean transformation in quantum mechanics* - Wigner symmetry operator for Galilean shift of position and momentum operators, explicit derivation of this operator

$$\hat{U}(\mathbf{v}, t) = e^{\frac{i}{\hbar}(\hat{\mathbf{p}}t - m\hat{\mathbf{r}})\mathbf{v}},$$

wave function transformation between two moving frames

$$\Psi_T(\mathbf{r}_T, t) = e^{\frac{i}{\hbar}(\frac{m\mathbf{v}^2}{2}t - m\mathbf{v}\mathbf{r})}\Psi(\mathbf{r}, t),$$

role of the local phase change in the wave function, resolution of the Lande's pseudoparadox, quantum Doppler effect

$$\frac{1}{\lambda'} = \frac{1}{\lambda} - \frac{mv}{h},$$

$$\nu' = \nu - \frac{v}{\lambda} + \frac{mv^2}{2h}.$$

6.2 Tutorial

6.3 Homework

1. *Dynamical symmetry in hydrogen atom, Runge-Lenz vector*[2] - For the Hamiltonian

$$\hat{H} = \frac{\hat{\mathbf{p}}^2}{2m} - \frac{\kappa}{r}$$

we introduce the Runge-Lenz vector

$$\hat{\mathbf{M}} = \frac{1}{2m}(\hat{\mathbf{p}} \times \hat{\mathbf{L}} - \hat{\mathbf{L}} \times \hat{\mathbf{p}}) - \kappa\frac{\mathbf{r}}{r}.$$

One can show that

$$[\hat{\mathbf{M}}, \hat{H}] = 0$$

$$\hat{\mathbf{L}} \cdot \hat{\mathbf{M}} = \hat{\mathbf{M}} \cdot \hat{\mathbf{L}} = 0$$

$$\hat{\mathbf{M}}^2 = \frac{2}{m}\hat{H}(\hat{\mathbf{L}}^2 + \hbar^2) + \kappa^2,$$

and

$$[\hat{L}_i, \hat{L}_j] = i\hbar\epsilon_{ijk}\hat{L}_k$$
$$[\hat{M}_i, \hat{L}_j] = i\hbar\epsilon_{ijk}\hat{M}_k$$
$$[\hat{M}_i, \hat{M}_j] = -2\frac{\hat{H}}{m}i\hbar\epsilon_{ijk}\hat{L}_k.$$

We consider bound states subspace of the Hilbert space with $E < 0$ and perform the rescaling of the Runge vector

$$\hat{\mathbf{M}}' = \sqrt{-\frac{m}{2\hat{H}}}\hat{\mathbf{M}}$$

and obtain the SO(4) commutator algebra

$$[\hat{L}_i, \hat{L}_j] = i\hbar\epsilon_{ijk}\hat{L}_k$$
$$[\hat{M}'_i, \hat{L}_j] = i\hbar\epsilon_{ijk}\hat{M}'_k$$
$$[\hat{M}'_i, \hat{M}'_j] = i\hbar\epsilon_{ijk}\hat{L}_k.$$

We introduce new operators

$$\hat{\mathbf{I}} = \frac{1}{2}(\hat{\mathbf{L}} + \hat{\mathbf{M}})$$

$$\hat{\mathbf{K}} = \frac{1}{2}(\hat{\mathbf{L}} - \hat{\mathbf{M}})$$

and we show that

$$[\hat{I}_i, \hat{I}_j] = i\hbar\epsilon_{ijk}\hat{I}_k$$
$$[\hat{K}_i, \hat{K}_j] = i\hbar\epsilon_{ijk}\hat{K}_k$$
$$[\hat{I}_i, \hat{K}_j] = 0.$$

The eigenstates of these operators and the Hamiltonian are $\{|im_ikm_k\rangle\}$ with eigenvalues

$$\hat{\mathbf{I}}^2 \to \hbar^2 i(i+1)$$
$$\hat{I}_z \to \hbar m_i$$
$$\hat{\mathbf{K}}^2 \to \hbar^2 k(k+1)$$
$$\hat{K}_z \to \hbar m_k$$

and

$$\hat{H} \to E_n = -\frac{m\kappa^2}{2\hbar^2 n^2},$$

where $n = 2i+1 \in N$ and $i = k$ was used from the orthogonality constraint. Discussion of symmetry and degeneracy of the hydrogen eigenstates. Based on W. Greiner, B. Müller *Quantum mechanics - symmetries.*

2. *Identity with* $\hat{\mathbf{M}}$ - Show that

$$\hat{\mathbf{M}}^2 = \frac{2}{m}\hat{H}(\hat{\mathbf{L}}^2 + \hbar^2) + \kappa^2.$$

3. *One of the commutator involving* $\hat{\mathbf{M}}$ *and* $\hat{\mathbf{L}}$ - Show that

$$[\hat{M}_1, \hat{L}_2] = i\hbar\hat{M}_3.$$

4. *One of the commutator involving* $\hat{\mathbf{M}}$ *and* $\hat{\mathbf{L}}$ - Show that

$$[\hat{M}_1, \hat{L}_1] = 0.$$

5. *For ambitious students* - Prove by yourself all equations presented in the problem 1.

[1] Shifted to the tutorial section.

[2] This is interesting problem related with the symmetry of the hydrogen atom. Please consider it as an extra, not obligatory exercise. Nevertheless, I recommend to work on it.

7 Week VII

7.1 Lecture

7.2 Tutorial

1. *Parity and spherical harmonics* - Discuss how spherical harmonics are transformed under the parity operation.

2. *Permanent electric dipole moment* - Discuss under which condition a permanent (spontaneous) dipole electric moment occurs in quantum mechanics. Consider linear Stark effect in $n = 2$ excited state in hydrogen.

3. *Antiunitary operators* - Let $\hat{A}$ is an antiunitary operator and $|\tilde{u}\rangle = \hat{A}|u\rangle$ and $|\tilde{v}\rangle = \hat{A}|u\rangle$. Show that $\langle\tilde{u}|\tilde{v}\rangle = \langle v|u\rangle = \langle u|v\rangle^*$.

4. *Antiunitary operator acting on bra* - How to define an action of the antiunitary operator $\hat{B}$ on a bra vector (to the left)
$$\langle v|\hat{B} = ?$$

5. *Adjoint to antiunitary operator* - How to define an adjoint operator $\hat{B}^\dagger$ to an antiunitary operator $\hat{B}$?

8 Week VIII

8.1 Lecture

&3. *Non-equivalent representations of momentum operators in quantum mechanics* - Position and momentum operators in quantum mechanics and their commutator, explicit form of these operators in position representation, momentum operator defined with respect to an arbitrary function, $\hat{x} = x$, $\hat{p} = -i\hbar d/dx + \chi(x)$, invariance of canonical commutation relations, transformation of the base $\{|x\rangle\}$ by multiplying by the phase factor $\exp(ig(x)/\hbar)$, where $g(x) = \int^x \chi(y)dy$, unitary change of the base, higher dimensional generalization, path independence of the phase $g(\mathbf{r}) = \int^{\mathbf{r}} \chi(\mathbf{r}')d\mathbf{r}'$, rotationless of the function $\nabla \times \chi(\mathbf{r}) = 0$, non-unique method in non-compact spaces.

&4. *Electromagnetic gauge representations in quantum mechanics* - reminder of scalar and vector potentials in classical electrodynamics, gauge freedom in classical electrodynamics, some popular gauges, incorporation of electromagnetic field in quantum mechanics, minimal coupling prescription, mechanical momentum vs. dynamical momentum, change of the wave function and states by adding the vector potential, electromagnetic gauge transformations in quantum mechanics.

8.2 Tutorial

1. *Product of unitary and antiunitary operators* - Let $\hat{\Psi} = \hat{\Theta}\hat{U}$, where $\hat{U}$ is an unitary operator and $\hat{\Theta}$ is an antiunitary operator. Show that $\hat{\Psi}$ is antiunitary.

2. *Product of two antiunitary operators* - Let $\hat{\Psi}$ and $\hat{\Theta}$ are antiunitary operators. Show that $\hat{U} = \hat{\Psi}\hat{\Theta}$ is unitary.

3. *Base dependence in representing an antiunitary operator* - Let $\hat{K}$ is a complex conjugation operator. Show that $\hat{K}$ is not independent of the phase of the basis vectors in terms of which it is defined.

4. *Rotation of a spin around one of the coordinate axis* - For the spin rotation operator with the angle π around the axis y,
$$\hat{U} = e^{-i\frac{\pi}{\hbar}\hat{S}_y},$$
show that $\hat{U}\hat{S}_x = -\hat{S}_x\hat{U}$ and $\hat{U}\hat{S}_z = -\hat{S}_z\hat{U}$.

8.3 Homework problems

1. *Time reversal and spherical harmonics* - Discuss how spherical harmonics are transformed under the time reversal operation.

2. *Rotation operator for fermions* - Find an explicit form (in terms of two by two matrices) of the spin rotation operator $\hat{U}(\phi\ \mathbf{n})$ for spin 1/2 particles. Show that $\hat{U}(2\pi\ \mathbf{n}) = -1$. ϕ is the rotation angle around the $\mathbf{n}$ direction.

9 Week IX

9.1 Lecture

&5. *Aharonov-Bohm effect* - model of infinite solenoid, absence of magnetic induction outside the solenoid tube, motion of a charge quantum particle outside the tube, relative phase of the wave functions and its dependence on the magnetic flux, unit of quantum flux.

&6 *Dirac magnetic monopole* - history of a magnetic monopole and the consideration of Dirac, theorem of non-existence of the single vector potential corresponding to the magnetic monopole, Wu and Yang consideration about the magnetic monopole, two different vector potentials covering the whole sphere in 3-dimensional space, gauge transformation between these potentials, quantization of the magnetic monopole due to single valuedness of the wave function, topological character of this quantization.

IV. Berry phases and topological states inn quantum mechanics

&1. *Adiabatic approximation* - adiabatic processes and adiabatic invariants in classical mechanics, two different time scales, to be continued ...

9.2 Tutorial

1. *Model of quantum harmonic crystal* - Detailed solution of the quantum harmonic crystal model in one dimension with periodic boundary condition: rising operators in lattice space, lattice Fourier transformation, Bogoliubov-Valatin diagonalization.

2. *Ferromagnet - a prominent exception* - The Heisenberg model, rotational symmetry of the Heisenberg model, exact ferromagnetic ground state without rotational symmetry, definition of orientation vector and its classical behavior in the thermodynamic limit, orthogonality of different oriented ferromagnetic states in the thermodynamic limit, symmetry breaking and classical behavior, low energy excitations of ferromagnets, quadratic dispersion of magnons, spin-waves.

3. *Spin-wave (magnon) excitation spectrum* - Find a dispersion relation of the spin-wave excitations around the ferromagnetic ground state of $d = 1$ Heisenberg model.

9.3 Homework problems

1. *Model of quantum harmonic crystal - different approach* - Consider the model

$$H = \sum_{j=1}^{N} \frac{p_j^2}{2m} + \frac{\kappa}{2} \sum_{j=1}^{N} (x_j - x_{j+1})^2.$$

Introduce Fourier transforms $x_k = (1/\sqrt{N}) \sum_j e^{ikaj} x_j$ and $p_k = (1/\sqrt{N}) \sum_j e^{ikaj} p_j$ and show that

$$H = \frac{1}{2m} \sum_k p_k p_{-k} + 2\kappa \sum_k \sin^2(ka/2) x_k x_{-k}.$$

Check commutation relations between new operators. Introduce creation and annihilation operators

$$a_k = \sqrt{\frac{m\omega_k}{2\hbar}} (x_k + i \frac{p_{-k}}{m\omega_k})$$

$$a_k^\dagger = \sqrt{\frac{m\omega_k}{2\hbar}} (x_{-k} - i \frac{p_k}{m\omega_k}),$$

where $\omega_k = 2\sqrt{\kappa/m} |\sin(ka/2)|$ and show that

$$H = \sum_k \hbar\omega_k (a_k^\dagger a_k + \frac{1}{2}).$$

2. *Poor men's version of Hohenberg-Mermin-Wagner theorem, instability of $d = 1$ crystal* - Calculate the mean square deviation of the n-th ion from its equilibrium position at $T = 0$, i.e. $\langle 0|\hat{x}_n^2|0\rangle$, within the model of quantum harmonic crystal. Since the result is divergent it implies that no long-range order is possible in one-dimensional system.

3. *Correlation function in the model of quantum harmonic crystal* - Within the model of quantum harmonic crystal determine the correlation function $\langle 0|(\hat{x}_n - \hat{x}_{n-l})^2|0\rangle$ in the ground state. Discuss the nearest neighbor bond length at $l = 1$ and discuss the limit $l \to \infty$.

4. *Model of quantum harmonic crystal with two atoms unit cell* - Consider one dimensional model of harmonic crystal with two different ions of masses m_1 and m_2 placed in an alternative manner. Distances between atoms are a and the interaction is of harmonic (quadratic) type between nearest neighbor ions. Find the excitation spectrum of this system. Check that there are two branches of excitations one gapless (Goldstone) and the other gapped, with finite energy at $k = 0$. Check the limit $m_1 = m_2$.

5. *Spin-wave (magnon) excitation spectrum in d-dimensions* - Find a dispersion relation of the spin-wave excitations (collective superposition of states with only one spin flipped) around the ferromagnetic ground state of a Heisenberg model with the exchange interaction between spins localized on nearest neighbor sites of a hypercubic lattice with the lattice constant a in d-dimensions. Hint: repeat steps from tutorial problem but the discrete Fourier transform must be d-dimensional.

10 Week X

10.1 Lecture

10.2 Tutorial

3 days May's holiday

11 Week XI

11.1 Lecture

... cont., quantum mechanical examples of adiabatic processes: infinite quantum well and Born-Oppenheimer approximation, adiabatic theorem in quantum mechanics and its prove.

&2. *Berry (geometric) phases* - Anholonomy in case of periodic processes, example of pendulum on the Earth surface, Foucault pendulum and Hannay's angle, relation of this angle to solid angle, geometric phase in quantum mechanics, the approximate form of the wave function in case of adiabatic processes, definition of dynamical and geometric phases, condition on the geometric phase, expression on the geometric phase in case of the change of the Hamiltonian parameters, flux interpretation of geometric phase, Berry's potential, Berry's flux, is the geometric phase real? is the geometric phase measureable?

11.2 Tutorial

1. *Einstein's gedanken experiment with a rocket* - Consider a rocket in an empty space and subjected to an acceleration equal to g. Suppose that inside the rocket there is a single quantum object, described by a Schrödinger equation with a confining potential $V(x, t)$, e.g. the rocket walls, in the laboratory frame. Find the Schrödinger equation in a reference frame co-moving with the rocket. Interpret this result.

2. *Gauge transformation in quantum mechanics* - Check by explicit calculation that the form of the

Schrödinger equations before and after the gauge transformation are the same.

3. *Quantum particle in uniform electric field* - Solve the problem of a quantum particle moving in a static uniform electric field $\mathbf{E} - E_0\mathbf{e}_x$. Solve the problem in: a) *static gauge* with $V = -E_0 x$, $\mathbf{A} = 0$, and b) *dynamic gauge* with $V = 0$ and $\mathbf{A} = -E_0 t\mathbf{e}_x$. Using these solutions, obtain solutions in the other gauges by taking a gauge transformation with $\chi = -E_0 xt$ scalar function.

11.3 Homework problems

1. *Quantum particle in a gravity field* - Solve a problem of a quantum particle with mass m falling in a uniform gravity field $V = mgz$ for $z > 0$, and assuming that for $z \leqslant 0$ the potential is of infinite height (hard wall potential). Discuss an energy quantization and a motion of a classical (gaussian) wave packet. Compare to results in an infinite space with the uniform gravity field, i.e. without the hard wall boundary. Hint: Am. J. Phys. **67**, 776 (1999), arxiv:2009.03744.

2. *Gauge invariant density, current, and continuity equation* - For a quantum particle with charge in the presence of an electromagnetic field find (guess) forms for the particle density and the current density, such that they are gauge invariant. Check if the continuity equation is gauge invariant as well.

12 Week XII

12.1 Lecture

&3. *Aharonov-Bohm phase as a Berry phase* - reinterpretation of the Aharonov-Bohm geometry in terms of adiabatic change of the system and interpretation of the magnetic flux as a geometric phase.

&4. *Emergent of a Berry monopole in a two level system* - generic form of a zero dimensional, two-level quantum mechanical Hamiltonian, unique eigenvalues and non-unique eigenvectors, necessity of using two gauges (e.g. north and south) determination of the Berry gauge dependent potential vector and the Berry gauge independent flux, magnetic monopole interpretation of the Berry vector potentials, a monopole at the degeneracy point in the Hamiltonian parameter space, emergence of the gauge structure in the adiabatically changed two level system.

12.2 Tutorial

1. *DC Josephson effect* - Using a simplified two-state model due to Feynman derive the Josephson equation on the tunneling current $J = J_0 \sin(\theta_2 - \theta_2)$ between two superconductors with fixed phases of their wave functions.

2. *AC Josephson effect* - Using a simplified two-state model due to Feynman derive the Josephson equation on the tunneling current between two superconductors with fixed phases of their wave functions which are biased by the gate voltage $V(t)$. Analyze in details the case where $V(t) = V_0$.

12.3 Homework problems

1. *Gauge invariant current density in superconductors* - Assuming the wave function as $\Psi(\mathbf{r}, t) = \sqrt{n(\mathbf{r}, t)}e^{i\theta(\mathbf{r},t)}$ and show that the current density is $\mathbf{J} = qn\mathbf{v}$, where $\mathbf{v} = \frac{\hbar}{m}\nabla\theta - \frac{q}{m}\mathbf{A}$. Check gauge invariance.

2. *AC Josephson effect - Shapiro steps* - Using a simplified two-state model due to Feynman derive the Josephson equation on the tunneling current between two superconductors with fixed phases of their wave functions which are biased by the gate voltage $V(t)$. Analyze in details the case where $V(t) = V_0 + V_1 \cos(\omega t)$.

13 Week XIII

13.1 Lecture

V. Scattering Theory

&1. *Introduction to scattering experiments* - typical scattering geometry, conservation laws in scattering experiments, elastic and inelastic scatterings, types of scattering experiments.

&2. *Scattering cross section* - incoming current and scattered current and their units, definition of differential and total cross sections, geometrical interpretation of the total cross section.

&3. *General theory of scattering - Lippmann-Schwinger equation* - derivation of a formal solution of the Schrödinger equation for continuous energies in term of Lippmann-Schwinger equation.

13.2 Tutorial

1. *SQUID - Superconducting QUantum Interference Device* - Consider two superconductors forming a loop with two Josephson junctions. Derive the formula for the current as a function of the magnetic flux inside the loop.

2. *Berry phase in the Born-Oppenheimer approximation* - Consider two-particle hamiltonian

$$\hat{H} = \frac{\hat{\mathbf{P}}}{2M} + \frac{\hat{\mathbf{p}}}{2m} + V(\mathbf{R}, \mathbf{r}),$$

where small and great letters correspond to light and heavy particles. In the limit $M \gg m$ one can take an ansatz on the wave function

$$\psi_n(\mathbf{R}, \mathbf{r}) = \phi_n(\mathbf{R})\xi_n(\mathbf{R}, \mathbf{r}),$$

where the eigen-problem for fast degrees of freedom (m)

$$\hat{h}(\mathbf{R})|n\mathbf{R}\rangle = \epsilon_n(\mathbf{R})|n\mathbf{R}\rangle$$

or

$$\hat{h}(\mathbf{R})\xi_n(\mathbf{R},\mathbf{r}) = \epsilon_n(\mathbf{R})\xi_n(\mathbf{R},\mathbf{r}),$$

depends on $\mathbf{R}$ only parametrically. Show that the eigen-problem for for the slow degrees of freedom (M) is described by the Hamiltonian

$$\hat{H}_{\text{eff}} = \frac{1}{2M}(\hat{\mathbf{P}} + \hbar\mathbf{A}_B)^2 + \epsilon_n(\mathbf{R}),$$

where $\mathbf{A}_B = i\int d_3r\xi_n(\mathbf{R},\mathbf{r})^*\nabla_{\mathbf{R}}\xi_n(\mathbf{R},\mathbf{r})$ is the Berry phase. Interpret these results.

13.3 Homework problems

1. *Beyond the adiabatic limit* - Taking the wave function expansion

$$\Psi_n(x,t) = \psi_n(x,t)e^{i\Theta_n(t)}e^{i\gamma_n(t)} +$$

$$+\epsilon\sum_{m\neq n} c_m(t)\psi_m(x,t)$$

check the correctness of the expression for the geometric phase up to the first order in the ϵ.

2. *Expanding adiabatically quantum well* - Calculate the geometric phase γ_n in the problem of infinite quantum well in one dimension if the well expands adiabatically from L_1 to L_2. If the expansion happens at a constant rate $dL/dt = v$ determine the dynamic phase Θ_n. If the well contracts to the original size, what is the Berry's phase? Make comments on these partial results.

3. *Particle in a rotating magnetic field* - An external magnetic field changes in time as

$$\mathbf{B}(t) = \begin{pmatrix} B_0\sin\alpha\cos\omega t \\ B_o\sin\alpha\sin\omega t \\ B_0\cos\alpha \end{pmatrix}.$$

Assume that at $t = 0$ the particle's spin points along the magnetic field. Check that the exact solution is in the form

$$\chi(t) =$$

$$\begin{pmatrix} (\cos(\lambda t/2) + i\frac{\omega_1+\omega}{\lambda}\sin(\lambda t/2))\cos(\alpha/2)e^{-i\omega t/2} \\ (\cos(\lambda t/2) + i\frac{\omega_1-\omega}{\lambda}\sin(\lambda t/2))\sin(\alpha/2)e^{i\omega t/2} \end{pmatrix},$$

where $\omega_1 = qB_0/m$ and $\lambda = \sqrt{\omega^2+\omega_1^2+2\omega\omega_1\cos\alpha}$. Compute the probability that the particle's spin will be anti-parallel to the magnetic field. Find the adiabatic conditions under which this probability vanishes. Compute the Berry phase during a singe cycle of rotation of the magnetic field.

4. *Two level system - Berry phase* - For a two level system discussed in the lecture derive all results on Berryology in details.

14 Week XIV

14.1 Lecture

&4. *Resolvents, Green's functions and Lippmann-Schwinger equation* - definition of a resolvent for a given Hamiltonian $\hat{G}(E) = (E - \hat{H})^{-1}$, application of the η trick, $E \to E + i\eta$ with $\eta \to 0^+$, formulation of the Lipman-Schwinger equation using the resolvent, formal solution of the Shrödinger equation by using $\hat{G}(E)$, relation of the η trick with the retarded boundary condition, formulation of the problem in terms of a time dependent Schrödinger equation and its solution by retarded Green's function, prove of the relation between the retarded boundary (initial) conditions with the $\eta \to 0^+$ procedure.

&5. *Formal solution of the Lippmann-Schwinger equation* - iterative solution to Lippmann-Schwinger equation, summation of the geometric progress, definition of the t-matrix operator (transition matrix), t-matrix as an effective scattering potential, Lippmann-Schwinger equation for the wave function, Born series for the wave function and for the t-matrix, multiple scattering interpretation of the Born series expansion.

14.2 Tutorial

1. *Phase of the Bloch function* - Check the invariance of the Schroedinger equation with a periodic potential if we perform the local in k-space phase transformation

$$\psi_{n\mathbf{k}}(\mathbf{r}) \to \psi'_{n\mathbf{k}}(\mathbf{r}) = e^{i\phi_n(\mathbf{k})}u_{n\mathbf{k}}(\mathbf{r})e^{i\mathbf{kr}}.$$

2. *Berry vector potential / connection for Bloch functions* - define the Berry connection $\mathbf{A}_{n\mathbf{k}} = -i\langle u_{n\mathbf{k}}|\nabla_{\mathbf{k}}u_{n\mathbf{k}}\rangle$ and show how it transforms under the local in k-space phase transformation introduced above. Introduce the Berry field /curvature for Bloch functions $\mathcal{F}_{n\mathbf{k}} = \nabla_{\mathbf{k}}\times\mathbf{A}_{n\mathbf{k}}$ and find an explicit expression that $\mathcal{F}_{n\mathbf{k}} = -i\langle\nabla_{\mathbf{k}}u_{n\mathbf{k}}|\times|\nabla_{\mathbf{k}}u_{n\mathbf{k}}\rangle$.

3. *position operator in Bloch space functions* - Show for a single band that the position operator in k-space in the presence of the periodic potential takes the form $\hat{\mathbf{r}} = i\nabla_{\mathbf{k}} - \mathbf{A}_{n\mathbf{k}}$.

4. *Equation of motion for momentum operator* - Show for a single band that the momentum operator satisfies

$$\frac{d\pi}{dt} = -q\nabla_{\mathbf{r}}\phi(\mathbf{r}) + q\mathbf{v}\times\mathbf{B},$$

where ϕ is the scalar electric potential, $\mathbf{B}$ is the magnetic induction, and q is the charge.

5. *Equation of motion for the position operator* - Show for a single band that the position operator satisfies

$$\frac{d\mathbf{r}}{dt} = \frac{1}{\hbar}\nabla_{\mathbf{k}}E(\mathbf{k}) + \frac{d\mathbf{k}}{dt}\times\mathcal{F}_{\mathbf{k}}.$$

The second term is called an anomalous velocity. It drives the anomalous Hall effect, a current perpendicular to the electric field.

14.3 Homework problems

1. *Particle on a ring pierced by a magnetic field* - A charged q particle is moving along a circle of radius R around a very narrow infinite solenoid with a magnetic flux Φ. The circle is perpendicular to the solenoid. Taking the vector potential inside the ring $\mathbf{A} = \frac{\Phi}{2\pi R}\mathbf{e}_\phi$ show that the eigenenergies are $E_n = \frac{\hbar^2}{2mR^2}(\Phi/\Phi_0 - n)^2$, where $\Phi_0 = 2\pi\hbar/q$. Interpret the quantum number n. What are the corresponding eigenstates? How the ground state and exited states change when Φ increases/decreases? Find the current density of those states and discuss it change with Φ.

2. *Wilczek-Zee phase* - Consider an M dimensional $\mathbf{R}(t) = (R_1(t), ..., R_M(t))$ parameter dependent Hamitlonian $\hat{H}(\mathbf{R}(0))$ with r-fold degenerate energy $E_n(\mathbf{R}(0))$

$$\hat{H}(\mathbf{R}(0))|\psi_{na}(\mathbf{R}(0))\rangle = E_n(\mathbf{R}(0))|\psi_{na}(\mathbf{R}(0))\rangle.$$

Let the initial state is $|\psi(0)\rangle = |\psi_{nb}(\mathbf{R}(0))\rangle$ for some fixed b.

Check that during an adiabatic evolution the state is

$$|\psi(t)\rangle = e^{-\frac{i}{\hbar}\int_0^t E_n(\mathbf{R}(t'))dt'} \sum_{a=1}^{r} U^{(n)}_{ab}(t)|\psi_{na}(\mathbf{R}(t))\rangle,$$

where $U^{(n)}_{ab}$ is a unitary $r \times r$ matrix operator satisfying

$$\left((\hat{U}^{(n)})^{-1}\frac{d\hat{U}^{(n)}}{dt}\right)_{ab} =$$
$$= -\langle\psi_{na}(\mathbf{R})|\nabla_{\mathbf{R}}\psi_{nb}(\mathbf{R})\rangle \cdot \frac{d\mathbf{R}(t)}{dt},$$

with $\hat{U}(0) = \hat{1}$. Define a matrix valued Berry vector potential

$$\mathbf{A}_{ab}(n, \mathbf{R}) = i\langle\psi_{na}(\mathbf{R})|\nabla_{\mathbf{R}}\psi_{nb}(\mathbf{R})\rangle,$$

where $(A_i)_{ab}(n, \mathbf{R})$ is a Hermitian $r \times r$ matrix and $i = 1, ..., M$.

Check that after a cyclic evolution $\mathbf{R}(0) = \mathbf{R}(T)$ on a closed contour C in the parameter space the solution on the matrix U is

$$\hat{U}^{(n)}(C) = T_C e^{i\oint_C \mathbf{A}(n,\mathbf{R})\cdot d\mathbf{R}},$$

where T_C is a chronological ordering operator on the contour C. Check that for non-degenerate case $r = 1$ it reproduces the Berry geometric phase. $\hat{U}^{(n)}(C)$ is called a non-abelian Wilczek-Zee factor. Under the adiabatic evolution of degenerate spectrum the state vector rotates in the degeneracy subspace.

Consider a gauge unitary transformation

$$|\tilde{\psi}_{na}\rangle = \sum_{b=1}^{r} \Lambda_{ab}|\psi_{nb}\rangle,$$

where $\hat{\Lambda}$ is a unitary $r \times r$ matrix. Show that the Berry matrix valued vector potential transforms as

$$\tilde{\hat{A}}_i(n, \mathbf{R}) = \hat{\Lambda}(\mathbf{R})\hat{A}_i(n, \mathbf{R})\hat{\Lambda}^{-1}(\mathbf{R}) + \frac{\partial\hat{\Lambda}(\mathbf{R})}{\partial R_i}\hat{\Lambda}^{-1}(\mathbf{R}).$$

It transforms as a non-abelian potential in a non-abelian gauge field theory. Define the Berry intensity field tensor

$$\hat{\mathcal{F}}_{ij}(n, \mathbf{R}) = \partial_i\hat{A}_j(n, \mathbf{R}) - \partial_j\hat{A}_i(n, \mathbf{R}) +$$
$$+[\hat{A}_i(n, \mathbf{R}), \hat{A}_j(n, \mathbf{R})]$$

and check that it transforms as

$$\tilde{\hat{\mathcal{F}}}_{ij}(n, \mathbf{R}) = \hat{\Lambda}(\mathbf{R})\hat{\mathcal{F}}_{ij}(n, \mathbf{R})\hat{\Lambda}^{-1}(\mathbf{R}).$$

15 Week XV

15.1 Lecture

&6. *Formal solution of the scattering problem in terms of the Green's function* - Resolvents and Green's functions for noninteracting and interacting problems, density of states and its relation to the Green's function, formal solution for the resolvent in terms of the t-matrix, proof of the Friedel sum rule theorem, proof of the optical theorem, definition of the s-matrix in on-shell scattering and its relation to the t-matrix, to be continued ...

15.2 Tutorial

1. *Resolvent in one-level model* - Find the resolvent and the Green's function for a system with the Hamiltonian
$$\hat{H} = \epsilon^a|a\rangle\langle a|.$$

2. *Resolvent in two-level model* - Find the resolvent and the Green's function for a system with the Hamiltonian

$$\hat{H} = \epsilon^a|a\rangle\langle a| + \epsilon^b|b\rangle\langle b| + V|a\rangle\langle b + V^*|a\rangle\langle b|.$$

Find the corresponding perturbative series with respect to V. Find t-matrix series. Interpret results diagrammatically. This is an elementary introduction to Feynman diagrams.

3. *Green's function in $d = 3$* - Compute the Green's function $G_0(\mathbf{r}, \mathbf{r}'; E)$ for free particles in $d = 3$ dimensions.

4. *Friedel oscillations* - Find how the density of electrons oscillates far away from the localized impurity potential in three dimensional space.

15.3 Homework problems

1. *Green's function in d dimensions* - Compute the Green's function $G_0(\mathbf{r}, \mathbf{r}'; E)$ for free particles in $d = 1$, $d = 2$ (and arbitrary d if you are interested in) dimensions.

2. *Density of states in d dimensions* - The local density of states (LDOS) is defined as

$$\rho(\mathbf{r}; E) = -\frac{1}{\pi} \lim_{\mathbf{r}' \to \mathbf{r}} \text{Im } G_0(\mathbf{r}, \mathbf{r}'; E).$$

Compute this quantity in $d = 1$, 2 and 3 dimensions. Compare with results obtained on your Statistical Physics course.

3. *Single site model with only one discrete state* - Find t-matrix, Green'd function, scattering phase shift, screening charge in case of a one level ϵ model treating a shift V of the energy level as perturbation. The Hamiltonian is $\hat{H} = \epsilon|0\rangle\langle 0| + V|0\rangle\langle 0|$.

Solution:

The Green function is

$$G_0(z) = \frac{1}{z - \epsilon}, \tag{1}$$

where ϵ is the energy of this level. The DOS is $\rho_0(\omega) = \delta(\omega - \epsilon)$ and the occupation of this system is

$$n_0 = \int \rho_0(\omega) f(\omega) d\omega = \frac{1}{e^{\beta(\epsilon-\mu)} + 1}, \tag{2}$$

where μ is the chemical potential.

We perturb this system by shifting the energy by V. he the Green function is

$$G(z) = \frac{1}{z - \epsilon - V}, \tag{3}$$

the DOS is $\rho(\omega) = \delta(\omega - \epsilon - V)$, and the occupation of this system is

$$n = \int \rho_0(\omega) f(\omega) d\omega = \frac{1}{e^{\beta(\epsilon+V-\mu)} + 1}. \tag{4}$$

The change of the DOS is

$$\Delta\rho(\omega) = \delta(\omega - \epsilon - V) - \delta(\omega - \epsilon), \tag{5}$$

and the screening charge is obtained

$$Z_{\text{sc}} = n - n_0 = \frac{1}{e^{\beta(\epsilon+V-\mu)} + 1} - \frac{1}{e^{\beta(\epsilon-\mu)} + 1}. \tag{6}$$

At $T = 0$ it reduces to

$$Z_{\text{sc}} = \Theta(\mu - \epsilon - V) - \Theta(\mu - \epsilon). \tag{7}$$

Now we derive the same result within the scattering formalizm. For a scalar functions we have an identity

$$G = \frac{d}{d\omega} \ln G^{-1}, \tag{8}$$

which leads to

$$\rho(\omega) = -\lim_{z \to \omega + i0^+} \frac{1}{\pi} \text{Im} \frac{d}{d\omega} \ln G(z)^{-1}. \tag{9}$$

Hence the change of DOS is

$$\begin{aligned}
\Delta\rho(\omega) &= -\lim_{z\to\omega+i0^+} \frac{1}{\pi}\frac{d}{d\omega}\text{Im }\ln\frac{G(z)^{-1}}{G_0(z)^{-1}} \\
&= -\lim_{z\to\omega+i0^+} \frac{1}{\pi}\frac{d}{d\omega}\text{Im }\ln\frac{z-\epsilon-V}{z-\epsilon} \\
&= -\lim_{z\to\omega+i0^+} \frac{1}{\pi}\frac{d}{d\omega}\text{Im }\ln(1-\frac{V}{z-\epsilon}) \\
&= \lim_{z\to\omega+i0^+} \frac{1}{\pi}\frac{d}{d\omega}\text{Im }\ln\frac{1}{V}\frac{V}{1-\frac{V}{z-\epsilon}} \\
&= \lim_{z\to\omega+i0^+} \frac{1}{\pi}\frac{d}{d\omega}\text{Im }\ln\frac{1}{V}T(z) \\
&= \frac{1}{\pi}\frac{d}{d\omega}\phi(\omega),
\end{aligned} \tag{10}$$

where

$$T(z) = \frac{V}{1 - \frac{V}{z-\epsilon}} \tag{11}$$

is the "T-matrix"(T-scalar) here and $\phi(\omega)$ is the scattering phase shift given by the argument of $T(\omega)$.

Determination of the phase must take into account multivaluedness of the logarithmic function. Indeed from

$$\omega + i0^+ - \epsilon = |\omega - \epsilon| e^{i\pi\Theta(\epsilon-\omega)}, \tag{12}$$

$$\omega + i0^+ - \epsilon - V = |\omega - \epsilon - V| e^{i\pi\Theta(\epsilon+V-\omega)}, \tag{13}$$

we find

$$\begin{aligned}
\lim_{z\to\omega+i0^+} \frac{1}{V}T(\omega) &= \lim_{z\to\omega+i0^+} \frac{z-\epsilon}{z-\epsilon-V} \\
&= |\frac{\omega-\epsilon}{\omega-\epsilon-V}| e^{i\pi(\Theta(\epsilon-\omega)-\Theta(\epsilon+V-\omega))}.
\end{aligned} \tag{14}$$

Therefore,

$$\begin{aligned}
\lim_{z\to\omega+i0^+} \ln\frac{1}{V}T(z) &= \ln|\frac{\omega-\epsilon}{\omega-\epsilon-V}| \\
&+ i\pi(\Theta(\epsilon-\omega) - \Theta(\epsilon+V-\omega).
\end{aligned} \tag{15}$$

The imaginary part

$$\begin{aligned}
\phi(\omega) &= \pi[\Theta(\epsilon-\omega) - \Theta(\epsilon+V-\omega)] \\
&= \pi[\Theta(\omega-\epsilon-V) - \Theta(\omega-\epsilon)],
\end{aligned} \tag{16}$$

since $\Theta(-x) = 1 - \Theta(x)$, is just the scattering phase shift. Although the spectrum is discrete the T-matrix has a nontrivial phase. From the Friedel sum rule we obtain

$$Z_{\text{sc}} = \frac{1}{\pi}\phi(\mu) = \Theta(\mu - \epsilon - V) - \Theta(\mu - \epsilon), \tag{17}$$

which agrees with the result before.

The change of DOS is

$$\begin{aligned}
\Delta\rho(\omega) &= \frac{1}{\pi}\frac{d}{d\omega}\phi(\omega) \\
&= \frac{d}{d\omega}(\Theta(\epsilon-\omega) - \Theta(\epsilon+V-\omega)) \\
&= \delta(\omega-\epsilon-V) - \delta(\omega-\epsilon).
\end{aligned} \tag{18}$$

This agrees with results from direct method given at the beginning, c.f., Eq. (5). Hence the screening charge is correctly the same. Therefore, the Friedel sum rule works for one site (discrete) non-interacting system.

Checking the consistency of choosing the phase

$$x \pm i0^+ = |x| e^{\pm i\pi\Theta(-x)}.$$

We know that

$$\frac{1}{x \pm i0} = P\frac{1}{x} \mp i\pi\delta(x).$$

On the other hand

$$\begin{aligned} \frac{1}{x \pm i0} &= \frac{d}{dx}\ln(x \pm i0^+) \\ = \frac{d}{dx}\ln(|x|e^{\pm i\pi\Theta(-x)}) &= \frac{d}{dx}(\ln|x| \pm i\pi\Theta(-x)) \\ = P\frac{1}{x} \pm i\pi\frac{d}{dx}\Theta(-x) &= P\frac{1}{x} \mp i\pi\delta(-x) \\ &= P\frac{1}{x} \mp i\pi\delta(x). \end{aligned} \tag{19}$$

□

4. *Two degenerate levels model with only one level perturbed* - Consider the model with $\hat{H} = -t|0\rangle\langle 1| - t|1\rangle\langle 0| - v|1\rangle\langle 1|$. Find t-matrix, Green'd function, scattering phase shift, screening charge treating a shift v of the energy level as perturbation.

Solution:

The free Green function matrix is

$$\mathbf{G}_0(z) = \begin{pmatrix} z & t \\ t & z \end{pmatrix}^{-1} = \frac{1}{z^2 - t^2}\begin{pmatrix} z & -t \\ -t & z \end{pmatrix}, \tag{20}$$

where the on site energy $\epsilon = 0$ and $t > 0$ is the hopping amplitude between sites. In the perturbed case the second site onsite energy is changed by $-v$, so the scattering potential is

$$\mathbf{V} = \begin{pmatrix} 0 & 0 \\ 0 & -v \end{pmatrix}, \tag{21}$$

and the Green function is

$$\begin{aligned} \mathbf{G}(z) = \begin{pmatrix} z & t \\ t & z+v \end{pmatrix}^{-1} &= \\ = \frac{1}{z(z+v) - t^2}\begin{pmatrix} z+v & -t \\ -t & z \end{pmatrix}&. \end{aligned} \tag{22}$$

The perturbed Green function $\mathbf{G}$ has singularities at

$$\omega_{1,2} = \frac{1}{2}[-v \pm \sqrt{v^2 + 4t^2}], \tag{23}$$

and the free Green function $\mathbf{G}_0$ is singular at

$$\omega^0_{1,2} = \pm t. \tag{24}$$

To find DOS we need the trace of $\mathbf{G}$ and $\mathbf{G}_0$:

$$\begin{aligned} \text{Tr } \mathbf{G}(z) &= \frac{2z+v}{z(z+v) - t^2} = \\ &= \frac{2z+v}{\omega_1 - \omega_2}\left(\frac{1}{z - \omega_1} - \frac{1}{z - \omega_2}\right) \end{aligned} \tag{25}$$

Observing that $\omega_1 - \omega_2 = \sqrt{v^2 + 4t^2}$ we obtain

$$\text{Tr } \mathbf{G}(z) = \frac{2z+v}{\sqrt{v^2+4t^2}}\left(\frac{1}{z-\omega_1} - \frac{1}{z-\omega_2}\right), \tag{26}$$

and in the limit $z \to \omega + i0^+$

$$\begin{aligned} \text{Tr } \mathbf{G}(\omega) = \frac{2\omega+v}{\sqrt{v^2+4t^2}}\bigg(&P\frac{1}{\omega-\omega_1} - i\pi\delta(\omega-\omega_1) \\ &-P\frac{1}{\omega-\omega_2} + i\pi\delta(\omega-\omega_2)\bigg). \end{aligned} \tag{27}$$

With observation that $2\omega_{1,2} + v = \pm\sqrt{v^2+4t^2}$ the DOS is

$$\begin{aligned} \rho(\omega) &= -\frac{1}{\pi}\text{Im Tr } \mathbf{G}(\omega) \\ &= \delta(\omega - \omega_1) + \delta(\omega - \omega_2). \end{aligned} \tag{28}$$

The unperturbed DOS is

$$\rho(\omega) = \delta(\omega - \omega^0_1) + \delta(\omega - \omega^0_2), \tag{29}$$

and the change of DOS is

$$\begin{aligned} \Delta\rho(\omega) = \delta(\omega - \omega_1) &+ \delta(\omega - \omega_2) \\ -\delta(\omega - \omega^0_1) &- \delta(\omega - \omega^0_2). \end{aligned} \tag{30}$$

The screening charge is

$$\begin{aligned} Z_{\text{sc}} = \int d\omega \Delta\rho(\omega) f(\omega) &= \frac{1}{e^{\beta(\omega_1-\mu)}+1} + \frac{1}{e^{\beta(\omega_2-\mu)}+1} \\ &- \frac{1}{e^{\beta(\omega^0_1-\mu)}+1} - \frac{1}{e^{\beta(\omega^0_2-\mu)}+1} \end{aligned} \tag{31}$$

and at $T = 0$ reduces to

$$\begin{aligned} Z_{\text{sc}} = \Theta(\mu - \omega_1) &+ \Theta(\mu - \omega_2) \\ -\Theta(\mu - \omega^0_1) &- \Theta(\mu - \omega^0_2). \end{aligned} \tag{32}$$

Next we use scattering to determine the change of DOS and the screening charge. From the main tex we have

$$\begin{aligned} \Delta\rho(\omega) &= \lim_{z\to\omega+i0^+}\frac{1}{\pi}\frac{d}{d\omega}\text{Im Tr ln}[\mathbf{V}^{-1}(z)\mathbf{T}(z)] \\ &= \lim_{z\to\omega+i0^+}\frac{1}{\pi}\frac{d}{d\omega}\text{Im Tr ln}[\mathbf{1} - \mathbf{V}\mathbf{G}_0]^{-1} \\ &= -\lim_{z\to\omega+i0^+}\frac{1}{\pi}\frac{d}{d\omega}\text{Im Tr ln}[\mathbf{1} - \mathbf{V}\mathbf{G}_0]. \end{aligned} \tag{33}$$

The matrix

$$\mathbf{1}-\mathbf{VG}_0 = \\ = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} - \frac{1}{z^2-t^2}\begin{pmatrix} 0 & 0 \\ 0 & -v \end{pmatrix}\begin{pmatrix} z & -t \\ -t & z \end{pmatrix} \\ = \begin{pmatrix} 1 & 0 \\ -\frac{vt}{z^2-t^2} & 1+\frac{zv}{z^2-t^2} \end{pmatrix} \quad (34)$$

needs to diagonalized. There are two eigenvalues $\lambda_1 = 1$ and $\lambda_2 = (z(z+v)-t^2)/(z^2-t^2)$ and logarith of diagonal matrix is a matrix of logarithm of its eigenvalues. Since the trace is base independent we have

$$\Delta\rho(\omega) = -\lim_{z\to\omega+i0^+}\frac{1}{\pi}\frac{d}{d\omega}\text{Im }(\ln\lambda_1+\ln\lambda_2). \quad (35)$$

Now $\ln\lambda_1 = 0$ and

$$\lim_{z\to\omega+i0^+}\ln\frac{z(z+v)-t^2}{z^2-t^2} \\ = \lim_{z\to\omega+i0^+}(\ln(z^2+zv-t^2)-\ln(z^2-t^2)) \\ = \ln|(\omega-\omega_1)(\omega-\omega_2)| + i\pi(\Theta(\omega_1-\omega)+\Theta(\omega_1-\omega)) \\ -\ln|(\omega-\omega_1^0)(\omega-\omega_2^0)| - i\pi(\Theta(\omega_1^0-\omega)+\Theta(\omega_1^0-\omega)). \quad (36)$$

Therefore we find nonzero scattering phase shift

$$\text{Tr }\boldsymbol{\phi}(\omega) = \pi[\Theta(\omega-\omega_1)+\Theta(\omega-\omega_2) \\ -\Theta(\omega-\omega_1^0)+\Theta(\omega-\omega_2^0)]. \quad (37)$$

The change of DOS

$$\Delta\rho(\omega) = \frac{1}{\pi}\frac{d}{d\omega}\pi[\Theta(\omega-\omega_1)+\Theta(\omega-\omega_2) \\ -\Theta(\omega-\omega_1^0)+\Theta(\omega-\omega_2^0)] \\ = \delta(\omega-\omega_1)+\delta(\omega-\omega_2) \\ -\delta(\omega-\omega_1^0)-\delta(\omega-\omega_2^0), \quad (38)$$

in agreement with result (30). From the Friedel sum rule we get

$$Z_{\rm sc} = \frac{1}{\pi}\text{Tr }\boldsymbol{\phi}(\mu) = \Theta(\mu-\omega_1)+\Theta(\mu-\omega_2) \\ -\Theta(\mu-\omega_1^0)+\Theta(\mu-\omega_2^0), \quad (39)$$

which agrees with result (32). Therefore, the Friedel sum rule works for two site (matrix) noninteracting system as well. We also note that it is easy to generalize this two site model by perturbing asymmetrically both sites by potentials v_1 and v_2 as is presented next.

As a double check we can use Cauchy formula to determine explicitly the logarithm of a matrix function, i.e.

$$\ln(\mathbf{1}-\mathbf{VG}_0) = \frac{1}{2\pi i}\int_\Gamma \ln\zeta\ [\zeta\mathbf{1}-\mathbf{1}+\mathbf{VG}_0]^{-1}d\zeta, \quad (40)$$

where the contour Γ incloses all eigenvalues λ_1 and λ_2 and the function $\ln\zeta$ is analytic on and inside it. Then we compute

$$\ln(\mathbf{1}-\mathbf{VG}_0) = \\ = \frac{1}{2\pi i}\int_\Gamma \ln\zeta \begin{bmatrix} \zeta-1 & 0 \\ \frac{vt}{z^2-t^2} & \zeta-1-\frac{vz}{z^2-t^2} \end{bmatrix}^{-1} d\zeta \\ = \frac{1}{2\pi i}\int_\Gamma \ln\zeta \frac{1}{(\zeta-1)(\zeta-1-\frac{vz}{z^2-t^2})}\cdot \\ \begin{bmatrix} \zeta-1-\frac{vz}{z^2-t^2} & 0 \\ -\frac{vt}{z^2-t^2} & \zeta-1 \end{bmatrix} d\zeta. \quad (41)$$

Using the theorem of residua we can compute each matrix element independently and obtain

$$\ln(\mathbf{1}-\mathbf{VG}_0) = \begin{bmatrix} 0 & 0 \\ -\frac{t}{z}\ln(1+\frac{vt}{z^2-t^2}) & \ln(1+\frac{vz}{z^2-t^2}) \end{bmatrix}, \quad (42)$$

which agrees with the earlier result gives the correct trace as presented above.

5. *Two site model with general potentials* - Consider the model with $\hat{H} = -t|1\rangle\langle 2| - t|2\rangle\langle 1| + v_1|1\rangle\langle 1| + v_2|1\rangle\langle 2|$. Find t-matrix, Green'd function, scattering phase shift, screening charge treating a shift v of the energy level as perturbation.

The free Green function matrix is

$$\mathbf{G}_0(z) = \begin{pmatrix} z-\epsilon & t \\ t & z-\epsilon \end{pmatrix}^{-1} \\ = \frac{1}{(z-\epsilon)^2-t^2}\begin{pmatrix} z-\epsilon & -t \\ -t & z-\epsilon \end{pmatrix}, \quad (43)$$

where ϵ is the on site energy and $t > 0$ is the hopping amplitude between sites. In the perturbed case both sites are shifted by potentials v_1 and v_2 respectively, so the scattering potential is

$$\mathbf{V} = \begin{pmatrix} v_1 & 0 \\ 0 & v_2 \end{pmatrix}, \quad (44)$$

and the Green function is

$$\mathbf{G}(z) = \begin{pmatrix} z-\epsilon-v_1 & t \\ t & z-\epsilon-v_2 \end{pmatrix}^{-1} \\ = \frac{1}{(z-\epsilon_1)(z-\epsilon_2)-t^2}\begin{pmatrix} z-\epsilon_2 & -t \\ -t & z-\epsilon_1 \end{pmatrix}, \quad (45)$$

where we used $\epsilon_1 = \epsilon + v_1$ and $\epsilon_2 = \epsilon + v_2$.

The perturbed Green function $\mathbf{G}$ has singularities at

$$\omega_{1,2} = \frac{1}{2}[\epsilon_1+\epsilon_2 \pm \sqrt{(\epsilon_1-\epsilon_2)^2+4t^2}], \quad (46)$$

and the free Green function $\mathbf{G}_0$ is singular at

$$\omega_{1,2}^0 = \epsilon \pm t. \quad (47)$$

To find DOS we need the trace of $\mathbf{G}$ and $\mathbf{G}_0$:

$$\begin{aligned}\text{Tr }\mathbf{G}(z) &= \frac{2z-\epsilon_1-\epsilon_2}{(z-\epsilon_1)(z-\epsilon_2)-t^2} \\ &= \frac{2z-\epsilon_1-\epsilon_2}{\omega_1-\omega_2}\left(\frac{1}{z-\omega_1}-\frac{1}{z-\omega_2}\right)\end{aligned} \quad (48)$$

Observing that $\omega_1-\omega_2=\sqrt{(\epsilon_1-\epsilon_2)^2+4t^2}$ we obtain

$$\text{Tr }\mathbf{G}(z) = \frac{2z-\epsilon_1-\epsilon_2}{\sqrt{(\epsilon_1-\epsilon_2)^2+4t^2}}\left(\frac{1}{z-\omega_1}-\frac{1}{z-\omega_2}\right), \quad (49)$$

and in the limit $z\to\omega+i0^+$

$$\begin{aligned}\text{Tr }\mathbf{G}(\omega) = \frac{2\omega-\epsilon_1-\epsilon_2}{\sqrt{(\epsilon_1-\epsilon_2)^2+4t^2}}\Bigg(&P\frac{1}{\omega-\omega_1}-i\pi\delta(\omega-\omega_1) \\ &-P\frac{1}{\omega-\omega_2}+i\pi\delta(\omega-\omega_2)\Bigg).\end{aligned} \quad (50)$$

With observation that $2\omega_{1,2}-\epsilon_1-\epsilon_2=\pm\sqrt{v^2+4t^2}$ the DOS is

$$\begin{aligned}\rho(\omega) &= -\frac{1}{\pi}\text{Im Tr }\mathbf{G}(\omega) \\ &= \delta(\omega-\omega_1)+\delta(\omega-\omega_2).\end{aligned} \quad (51)$$

The unperturbed DOS is

$$\rho(\omega)=\delta(\omega-\omega_1^0)+\delta(\omega-\omega_2^0), \quad (52)$$

and the change of DOS is

$$\begin{aligned}\Delta\rho(\omega) &= \delta(\omega-\omega_1)+\delta(\omega-\omega_2) \\ &\quad -\delta(\omega-\omega_1^0)-\delta(\omega-\omega_2^0).\end{aligned} \quad (53)$$

The screening charge is

$$\begin{aligned}Z_{\text{sc}} = \int d\omega\Delta\rho(\omega)f(\omega) &= \frac{1}{e^{\beta(\omega_1-\mu)}+1}+\frac{1}{e^{\beta(\omega_2-\mu)}+1} \\ &\quad -\frac{1}{e^{\beta(\omega_1^0-\mu)}+1}-\frac{1}{e^{\beta(\omega_2^0-\mu)}+1}\end{aligned} \quad (54)$$

and at $T=0$ reduces to

$$\begin{aligned}Z_{\text{sc}} &= \Theta(\mu-\omega_1)+\Theta(\mu-\omega_2) \\ &\quad -\Theta(\mu-\omega_1^0)-\Theta(\mu-\omega_2^0).\end{aligned} \quad (55)$$

Next we use scattering to determine the change of DOS and the screening charge. From the main tex we have

$$\begin{aligned}\Delta\rho(\omega) &= \lim_{z\to\omega+i0^+}\frac{1}{\pi}\frac{d}{d\omega}\text{Im Tr ln}[\mathbf{V}^{-1}(z)\mathbf{T}(z)] \\ &= \lim_{z\to\omega+i0^+}\frac{1}{\pi}\frac{d}{d\omega}\text{Im Tr ln}[\mathbf{1}-\mathbf{VG}_0]^{-1} \\ &= -\lim_{z\to\omega+i0^+}\frac{1}{\pi}\frac{d}{d\omega}\text{Im Tr ln}[\mathbf{1}-\mathbf{VG}_0].\end{aligned} \quad (56)$$

The matrix

$$\begin{aligned}&\mathbf{1}-\mathbf{VG}_0 = \\ &= \begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix} - \\ &-\frac{1}{(z-\epsilon)^2-t^2}\begin{pmatrix}v_1 & 0\\ 0 & v_2\end{pmatrix}\begin{pmatrix}z-\epsilon & -t\\ -t & z-\epsilon\end{pmatrix} = \\ &= \begin{pmatrix}1-\frac{(z-\epsilon)v_1}{(z-\epsilon)^2-t^2} & \frac{v_1 t}{(z-\epsilon)^2-t^2}\\ \frac{v_2 t}{(z-\epsilon)^2-t^2} & 1-\frac{(z-\epsilon)v_2}{(z-\epsilon)^2-t^2}\end{pmatrix}\end{aligned} \quad (57)$$

needs to diagonalized. There are two eigenvalues

$$\begin{aligned}\lambda_\pm = \frac{1}{2}\Bigg[&2-\frac{(v_1+v_2)(z-\epsilon)}{(z-\epsilon)^2-t^2} \\ &\pm\sqrt{\frac{(v_1-v_2)^2(z-\epsilon)^2+4v_1v_2t^2}{((z-\epsilon)^2-t^2)^2}}\Bigg]\end{aligned} \quad (58)$$

and logarithm of diagonal matrix is a matrix of logarithm of its eigenvalues. Since the trace is base independent we have

$$\begin{aligned}\Delta\rho(\omega) &= -\lim_{z\to\omega+i0^+}\frac{1}{\pi}\frac{d}{d\omega}\text{Im }(\text{ln}\lambda_+ + \text{ln}\lambda_-) \\ &= -\lim_{z\to\omega+i0^+}\frac{1}{\pi}\frac{d}{d\omega}\text{Im ln}(\lambda_+\lambda_-).\end{aligned} \quad (59)$$

After some algebraic manipulation one can easily show that

$$\begin{aligned}\lambda_+\lambda_- &= \frac{(z-\epsilon)^2-(v_1+v_2)(z-\epsilon)+v_1v_2-t^2}{(z-\epsilon)^2-t^2} \\ &= \frac{(z-\omega_1)(z-\omega_2)}{(z-\omega_1^0)(z-\omega_2^0)}.\end{aligned} \quad (60)$$

Therefore,

$$\begin{aligned}&\lim_{z\to\omega+i0^+}\text{ln}(\lambda_+\lambda_-) \\ &= \text{ln}|(\omega-\omega_1)(\omega-\omega_2)|+i\pi(\Theta(\omega_1-\omega)+\Theta(\omega_1-\omega)) \\ &-\text{ln}|(\omega-\omega_1^0)(\omega-\omega_2^0)|-i\pi(\Theta(\omega_1^0-\omega)+\Theta(\omega_1^0-\omega)).\end{aligned} \quad (61)$$

Hence, we find nonzero scattering phase shift

$$\begin{aligned}\text{Tr }\boldsymbol{\phi}(\omega) = \pi[&\Theta(\omega-\omega_1)+\Theta(\omega-\omega_2) \\ &-\Theta(\omega-\omega_1^0)+\Theta(\omega-\omega_2^0)].\end{aligned} \quad (62)$$

The change of DOS

$$\begin{aligned}\Delta\rho(\omega) &= \frac{1}{\pi}\frac{d}{d\omega}\pi[\Theta(\omega-\omega_1)+\Theta(\omega-\omega_2) \\ &\quad -\Theta(\omega-\omega_1^0)+\Theta(\omega-\omega_2^0)] \\ &= \delta(\omega-\omega_1)+\delta(\omega-\omega_2) \\ &\quad -\delta(\omega-\omega_1^0)-\delta(\omega-\omega_2^0),\end{aligned} \quad (63)$$

in agreement with result (53). From the Friedel sum rule we get

$$\begin{aligned}Z_{\text{sc}} = \frac{1}{\pi}\text{Tr }\boldsymbol{\phi}(\mu) &= \Theta(\mu-\omega_1)+\Theta(\mu-\omega_2) \\ &\quad -\Theta(\mu-\omega_1^0)+\Theta(\mu-\omega_2^0),\end{aligned} \quad (64)$$

which agrees with result (55). Therefore, the Friedel sum rule works for general two site (matrix) non-interacting system as well.

16 Week XVI

16.1 Lecture

... continued, bound states and states from the continuum, Levinson's theorem and its prove, topological character of the Levinson's theorem.

&7. *Scattering amplitude* - Expansion of the Lippmann-Schwinger equation far away from the scattering potential center, definition of the scattering amplitude, relation of the scattering amplitude and the T-matrix, relation between η-trick, retarded boundary condition and purely outgoing boundary condition, outgoing spherical wave with modified amplitude, the scattering cross-section and the scattering amplitude, different formulations of the optical theorem.

&8. *Resonances, resonant states* - experimental evidence of resonance states in the cross-section, intuitive relation with quasi-bound states with a finite life-time, classification of possible solutions of the Schrödinger equation and their location on complex energy plane and complex momentum plane: i) continuum states, ii) bound states, iii) virtual states, iv) resonant states, v) antiresonance states, two Riemann sheets of the complex energy plane and the locations of the different solutions, properties of the resonances in space and in time, Bright-Wigner formula for resonances, mathematical origin for complex eigen-energies of resonances, difference between hermitian and self-adjoint operators, purely outgoing boundary condition as a source of non-self-adjointness.

16.2 Tutorial

1. *δ-Dirac potential* - Consider particles with mas m moving in one dimension. The potential is $V(x) = -V_)\delta(x)$, where $\delta(x)$ is a Dirac distribution. Solve this problem for bound states $E < 0$ and scattered states $E > 0$ within the wave function approach with proper boundary conditions at $x = 0$. Discuss results. Next, for scattered states $E > 0$ solve this problem within: a) t-matrix formalism, b) Lippmann-Schwinger formalism.

16.3 Homework problems

1. *Anderson-Fano-Friedrichs-Lee resonant model* - Consider the AFFL model

$$\hat{H} = \epsilon_0|0\rangle\langle 0| + \int_R dk\epsilon_k|k\rangle\langle k| +$$
$$+ \int dk_R V_k|0\rangle\langle k| + V_k^*|k\rangle\langle 0|.$$

Compute Green functions and find t-matrix. Discuss analytic structure of the t-matrix and its poles and a cut on both Riemann's sheets. For an explicit discussion assume that the DOS is constant $1/2D$ between $-D$ and D and zero otherwise and that $V_k = V_k^* = V$.

2. *Double δ-potential* - Consider a system in one dimension with the potential

$$V(x) = V_0[\delta(x + l) + \delta(x - l)],$$

with $V_0 > 0$. Assuming the purely outgoing boundary conditions, i.e. taking an ansatze for the solution

$$\psi_{\rm res}(x) = \begin{cases} Be^{-ikx} & \text{for } x < -l \\ Fe^{ikx} + Ge^{-ikx} & \text{for } -l < x < l \\ Ce^{ikx} & \text{for } l < x, \end{cases}$$

find equation(s) on k_n and energies $E_n = \hbar^2 k_n^2/2m$. By solving them numerically show that the complex solutions are admitted $E_n = \epsilon_n^r - i\Gamma_n/2$. Find them numerically, e.g. with Mathematica. These are resonances. Hint: arxiv:0705.1388.

3. *Double δ-potential - transition and reflection coeffcients* - Consider again a system in one dimension with the potential

$$V(x) = V_0[\delta(x + l) + \delta(x - l)],$$

with $V_0 > 0$. Assuming the boundary conditions with incoming wave from the left, i.e. taking an ansatze for the solution

$$\psi_{\rm res}(x) = \begin{cases} Ae^{ikx} + Be^{-ikx} & \text{for } x < -l \\ Fe^{ikx} + Ge^{-ikx} & \text{for } -l < x < l \\ Ce^{ikx} & \text{for } l < x, \end{cases}$$

derive transition $t(k) = C/A$ and reflection $r(k) = B/A$ coefficients. Show, that their divergence, i.e. when $A = 0$ (as in purely outgoing boundary condition, gives the same condition on k as in the former problem. Plot, e.g. with Mathematica, $t(E)$ for real $E = \hbar^2k^2/2m > 0$ and check if positions of maxima correlate with ϵ_n^r. Hint: arxiv:0705.1388.

17 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.