Lectures on Classical Fields and Quantum Mechanics. Part I

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Thème 4 — Simulation et optimisation
de systèmes complexes
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Abstract: These notes have been finished at INRIA during my visit of the project ONDES in January-February 2003. They correspond to a one-term course given at the University of Vienna in 2002 year. The aim of the notes is to give an introduction to Classical Field Theory and Quantum Mechanics for mathematicians. We start with the Lagrangian and Hamiltonian Theory of finite-dimensional systems and general nonlinear wave equations. Next we prove the Noether Theory of Invariants for the Fields and expose the Lagrangian form of the Maxwell Electrodynamics. Then we give a concise introduction of the Schrödinger Equation for the electron in the Maxwell Field: the equation describes the particle-like properties of cathode rays through the short-wave WKB-asymptotics. Finally, we apply the Schrödinger Equation to the derivation of spectrum of Hydrogen atom, dipole radiation and selection rules in a uniform magnetic field.

Key-words: Lagrange equations, invariants, Maxwell equations, Schrödinger equation, radiation, spectrum, Hydrogen, selection rules

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Les Champs Classique et Mécanique Quantique. Partie I

Résumé : Ces notes de cours ont été finalisées à l'INRIA pendant ma visite du Projet ONDES en Janvier-Février 2003. Elles correspondent à un cours d'un semestre à l'Université de Vienne en 2002. Le but de ces notes est une introduction à la Théorie Classique des Champs et Mécanique Quantique pour les mathématiciens. Nous commençons par la théorie de Lagrange et Hamilton pour des systèmes de dimension finie et des équations d'ondes non linéaires générales. Nous démontrons ensuite le théorème des Invariants de Noether pour les champs et exposons l'Électrodynamique de Maxwell dans la forme Lagrangienne. Nous introduisons enfin l'Équation de Schrödinger pour un électron soumis à un champ électromagnétique: l'équation permet de décrire les propriétés de type particule des rayons de cathode par l'intermédiaire des asymptotiques WKB pour les ondes courtes. Finalement, nous appliquons l'équation de Schrödinger pour la détermination de la spectre de l'atome d'Hydrogène, la radiation dipolaire et les règles de sélection dans le champ magnétique uniforme.

Mots-clés : équations de Lagrange, invariants, équations de Maxwell, équations de Schrödinger, radiation, spectre, Hydrogène, règles de sélection

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1 Lecture 1. Introduction

1.1 Missing "matter equation" and Quantum Mechanics

The Maxwell Theory (1865) describes perfectly the motion of charged particles in *given* electromagnetic fields and also the propagation of the electromagnetic waves generated by the *given* charge and current densities ρ, j. However, generally it cannot describe the evolution of the unknown densities and the fields since the *microscopic* evolution equation for the densities is missing. The representation of the densities as the motion of the charged particles does not help since the corresponding *mass density* μ is unknown (the ratio ρ/μ is unknown and even does not have a reasonable meaning since the ratio e/m takes different values for different elementary particles).

The situation is better only on the *macroscopic* level in the *simple* media with known electro- and magnetic permeability and conductivity since then the densities ρ, j are the *functions* of the fields (*Ohm* law etc). However this is not the case for the vacuum. Hence the Classical Electrodynamics is not sufficient to explain the structure of matter at the *microscopic* level.

Quantum Mechanics just provides various matter equations: Schrödinger, Klein-Gordon Eqns etc. The equations arise *inside* the Classical Electrodynamics, Thermodynamics, Optics and Atomic Physics from experimental observations of various aspects of the field-matter interaction and their theoretical interpretation. Let us sketch a history of the genesis.

1.1.1 Classical Electrodynamics, Thermodynamics and Optics

The cathode rays and the electron The cathode rays were discovered first in the vacuum tube by Crookes in 1870. The rays demonstrate the continuous charge motion in the vacuum in the presence of the Maxwell field. This is just the situation which is not covered by the Classical Electrodynamics.

The deflection of the cathode rays in a magnetic field has been observed by Hertz, Lenard, Perrin and many others.

Some physicists thought with Goldstein, Hertz, and Lenard, that this phenomenon is like light, due to vibrations of the ether or even that it is light of short wavelength. It is easily understood that such rays may have a rectilinear path, excite phosphorescence, and effect photographic plates. Others thought, with Crookes, J.J. Thomson, Perrin and others that these rays are formed by matter which is negatively charged and moving with great velocity, and on this hypothesis their mechanical properties, as well as the manner in which they become curved in a magnetic field, are readily explicable.

Perrin (1895) collected the cathode rays, obtaining a negative charge.

In 1897 J.J.Thomson showed that the rays also are deflected by an electrostatic field. He has systematized all previous observations and demonstrated the particle-like behavior of the rays which corresponds to the Newton equation with the Lorentz force,

$$a = \frac{e}{m}(E + v \times B), \qquad (L)$$

where $\frac{e}{m} < 0$. Respectively, he identified the cathode rays with a beam of particles with negative charge and introduced the name *the electron* for these particles. This study led to the first measurement of the ratio $\frac{e}{m}$ close to its present value.

Kauffmann [10] also observed the magnetic deflection of cathode rays and obtained a ratio $\frac{e}{m}$ which is close to the value of J.J.Thomson.

J.J.Thomson's identification of the cathode rays led to many fundamental problems concerning the size and the structure of the electron:
i) Abraham (1906) noted that the energy and mass of the electron are infinite if its radius is zero, he introduced the model of the *extended* electron and calculated its radius.
ii) The extended electron cannot be stable because of the electrostatic repulsion (Poincaré 1908).

So the Classical Electrodynamics has to be complemented with a *matter equation* which could describe i) the cathode rays and its *particle-like* behavior, and ii) the stability of the electron.

The black-body radiation In 1859 G.Kirchhoff stated the radiation law which predicts a special character of the spectral density of the light waves radiated by a black body at a fixed temperature. The light has been identified with the electromagnetic field by Maxwell in 1865. Hence, the Kirchhoff law concerns the spectrum of the equilibrium distribution of the electromagnetic field at a fixed temperature. Therefore it provides a deep indirect information on the interaction of the matter with the Maxwell field.

The experimental measurements have been performed by Tyndall in 1865, Crova in 1880, Langley in 1886, Weber in 1887, Paschen in 1895-1899. Most precise measurements were made in 1899 by Lummer and Pringscheim, and Kurlbaum and Rubens. They confirmed the Wien formula

$$I(\omega) \sim \omega^3 \exp(-\frac{a\omega}{T}) \qquad (W)$$

Note that the traditional reference to the *black* body just means that its equilibrium radiation coincides with the equilibrium Maxwell field since the absorption of the black body by definition is zero.

The comparison of (W) with the general equilibrium Boltzmann-Gibbs distribution $\exp(-\frac{E}{kT})$ (where k is the Boltzmann constant) suggests the famous Planck relation (1901)

$$E = \hbar\omega \qquad (P)$$

where E is the energy of the emitted "photon" and $\hbar = a/k \approx 1.05 \cdot 10^{-27} erg \cdot sec$ is the Planck constant. Using the relation, Planck adjusted the formula (W) as

$$I(\omega) \sim \omega^2 \frac{\exp(-\frac{a\omega}{T})}{1 - \exp(-\frac{a\omega}{T})}. \qquad (KP)$$

1.1.2 Optics and Atomic Physics

Photoeffect In 1887 Herz discovered the photoeffect (the "light electricity") as generation of the electric charge by the sun radiation. Later the photoeffect has been observed with different electromagnetic radiations by Stoletov, Elster, Geitel, Righi, Townsend, Rutherford, Compton and lots of others. The experimental observations gave the relation

$$\hbar\omega = E_{\rm el} - A, \qquad (E)$$

where $E_{\rm el}$ is the (maximal) energy of the photoelectrons detached from the metal by the light of the frequency ω.

In 1905 Einstein proposed the theory of the photoeffect [5]: he identified the identity (E) with the energy balance. Namely, Einstein
i) identified the quantity $\hbar\omega$ with the energy of the *absorbed* photon with frequency ω in accordance with the Planck relation (P) (which concerns the *emitted* photon !), and
ii) identified A with the *escape energy* of the metal.

This explanation treat the light as a collection of particle-like "photons" that cannot be explained by only using a wave picture of light and the classical representation of the electrons as particles.

Scattering of light by electrons In 1923 Compton, discovered that the scattered light has a wavelength λ' different from the wavelength λ of the incident light:

$$\lambda' - \lambda \sim \frac{2\hbar}{mc} \sin^2 \frac{\theta}{2}$$

where θ is the angle between the incident and scattered waves. Similarly to the photoeffect, the scattering also cannot be explained by only using a wave picture of light, where the wavelength does not change.

The atom nucleus and the atom stability In 1913 Rutherford discovered the atom nucleus in an experiment on the scattering of α-particles. This discovery suggested to him the classical model of the atom as a finite number of electrons moving around the point nucleus with positive charge. The electrons are governed by the classical Lorentz Eqn (L). However, the model is unstable due to the radiation of the rotating electrons in accordance with the Maxwell electrodynamics. Therefore, the Maxwell theory is insufficient to explain the stability of the atoms.

Atomic spectra and quantum transitions Atom spectra provide an extremely important information on the atom structure which gives new insight into the problem.

In 1885 Balmer has discovered the representation $\omega_{2n} = C\Big(\frac{1}{2^2} - \frac{1}{n^2}\Big)$ $(n \geq 3)$ for a spectral series in the Hydrogen atom spectrum. Later similar representations were found for another series by Lyman (1909) $\omega_{1n} = C\Big(1 - \frac{1}{n^2}\Big)$ $(n \geq 2)$, Paschen (1908) $\omega_{3n} = C\Big(\frac{1}{3^2} - \frac{1}{n^2}\Big)$ $(n \geq 4)$ and Brackett (1914) $\omega_{4n} = C\Big(\frac{1}{4^2} - \frac{1}{n^2}\Big)$ $(n \geq 5)$. Similar structure

$$\omega_{mn} = \omega_m - \omega_n, \qquad (R)$$

has been discovered by Rydberg (1900) for all the lines in the several series of the same elements. The importance of the observation was also stressed by Ritz (1908) so it is now commonly known as the *Rydberg-Ritz combination principle*, and the numbers ω_m are called the *terms*. In 1913 Niels Bohr rewrite (R) in the form

$$\hbar\omega_{mn} = E_m - E_n \qquad (B)$$

suggested by the comparison of the formulas (R) and (E). Moreover, Bohr interpreted (B) generalizing the Planck and Einstein ideas:

I. (B) means the energy balance in the transition

$$|E_m\rangle \mapsto |E_n\rangle.$$

between the *stationary states* $|E_m\rangle$ and $|E_n\rangle$ of the electron in the atom with the energies E_m, E_n.

II. the transition is followed by the radiation of light with the frequency ω_{mn} and the energy $\hbar\omega_{mn}$ in accordance with the Planck resp. Einstein identification of the quantum $\hbar\omega$ with the energy of the emitted resp. absorbed photon.

The role of the Planck constant $\hbar$ cannot be explained by the Maxwell theory as well as the discreteness of energies E_n of the stationary states. The discreteness of the energies means a restriction to certain *stable* orbits of the electron in the atom.

"Old" quantum theory In 1913 Debye stated the *quantum rule* for the determination of stable *periodic* orbits of the electrons in the atom,

$$\Delta S = 2\pi n\hbar, \quad n = 1, 2, 3, ... \qquad (D)$$

where ΔS is the action integral corresponding to the time-periodic orbit of the electron. The rule was motivated by the Ehrenfest idea of adiabatic invariance. In 1916 Sommerfeld and Wilson extended the rule to more general *quasiperiodic* orbits. The quantum rules allowed to find the Hydrogen spectral terms $\omega_n = \frac{C}{n^2}$, $n = 1, 2, ...$ which exactly agree with the Lyman, Balmer series etc.

Atoms in magnetic fields In 1896 Zeeman discovered the splitting of the spectral lines of atoms in a magnetic field. Lorentz explained the splitting by the Maxwell theory in the simplest case of the *normal* Zeeman effect when the line ω splits into three lines: ω and $\omega = \omega \pm \Delta\omega$, where $\Delta\omega$ is proportional to the magnetic field. However the explanation of the general *anomalous* Zeeman effect cannot be deduced from the Maxwell theory: for example, the double-splitting for the spectra of the alkali atoms.

The Maxwell theory predicts a unique value r for the gyromagnetic ratio μ/M, where μ resp. M is the magnetic resp. mechanical momentum of the electron in the atom In 1915 Einstein and de Haas first measured the gyromagnetic ratio, however the observed ratio was $2r$ i.e. two times larger than the theoretical.

In 1921 Stern and Gerlach observed the double-splitting of a beam of silver atoms in a strong nonuniform magnetic field. It also means the splitting of the stationary state of the atom in two states with different gyromagnetic ratios μ/M which again contradicts the Maxwell theory.

Wave-particle duality for free particles In 1911 Einstein suggested a possible description of matter by waves in parallel to the particle-wave duality of light which is demonstrated by the Maxwell theory and the photoeffect (E). In 1922 de Broglie in his PhD Thesis realized the Einstein idea for the free particle beam with the energy-momentum vector $(E, \mathbf{p})$. Namely:
i) the beam is identified with the plain wave by the following "wave-particle" relation:

$$\text{"free particles"}(E, \mathbf{p}) \leftrightarrow \psi(t, \mathbf{x}) = e^{i(\mathbf{kx} - \omega t)}$$

ii) the identity holds

$$(E, \mathbf{p}) = \hbar(\omega, \mathbf{k}) \qquad (dB)$$

which follows from the Einstein relativity principle and $(P1)$.
iii) (dB) implies the famous de Broglie relation for the wave length $\lambda = 2\pi/|\mathbf{k}|$,

$$\lambda = \frac{2\pi\hbar}{|\mathbf{p}|} .$$

It implies also the relativistic dispersion relation

$$\frac{\hbar^2\omega^2}{c^2} = \hbar^2\mathbf{k}^2 + m^2c^2,$$

as for relativistic particles the energy E satisfies the relation

$$\frac{E^2}{c^2} = \mathbf{p}^2 + m^2c^2, \qquad (1.1)$$

where c is the speed of light.
iv) For small values of $|\mathbf{p}| \ll mc$ the nonrelativistic approximation holds,

$$E = \sqrt{\mathbf{p}^2c^2 + m^2c^4} \approx mc^2 + \frac{\mathbf{p}^2}{2m} . \qquad (1.2)$$

Dropping here "unessential" additive constant mc^2, one get the nonrelativistic dispersion relation

$$\hbar\omega = \frac{\hbar^2\mathbf{k}^2}{2m}\,.$$

The dispersion relations imply the *free* Klein-Gordon resp. Schrödinger equations for corresponding wave function ψ from (WP):

$$\frac{1}{c^2}(i\hbar\partial_t)^2\psi(t,\mathbf{x}) = [(-i\hbar\nabla_{\mathbf{x}})^2 + m^2c^2]\psi(t,\mathbf{x}), \qquad (KG_0)$$

$$i\hbar\partial_t\psi(t,\mathbf{x}) = \frac{1}{2m}(-i\hbar\nabla_{\mathbf{x}})^2\psi(t,\mathbf{x}). \qquad (S_0)$$

Wave equations for bound particles In 1925-1926 Klein, Gordon and Schrödinger extended de Broglie's wave equation to the bound electron in an external Maxwell field. Namely, the *free* equations (KG_0) resp. (S_0) formally follow from the energy-momentum relations (1.1) resp. (1.2) by the substitutions $E \mapsto i\hbar\partial_t$, $\mathbf{p} \mapsto -i\hbar\nabla_{\mathbf{x}}$. For the electron in the external electrostatic potential $\phi(t,\mathbf{x})$ and static magnetic vector-potential $A(t,\mathbf{x})$, the (conserved) energy E is given by $(E-e\phi(t,\mathbf{x}))^2/c^2 = (\mathbf{p}-\not{e}A(t,\mathbf{x}))^2 + m^2c^2$, where e is the charge of the electron and $\not{e} := e/c$. Then Klein, Gordon and Schrödinger generalized (KG_0) by

$$\frac{1}{c^2}(i\hbar\partial_t - e\phi(t,\mathbf{x}))^2\psi(t,\mathbf{x}) = (-i\hbar\nabla_{\mathbf{x}} - \not{e}A(t,\mathbf{x}))^2\psi(t,\mathbf{x}) + m^2c^2\psi(t,\mathbf{x}). \qquad (KG)$$

Schrödinger generalized also the nonrelativistic approximation (S_0) by means of $E - e\phi(t,\mathbf{x}) = (\mathbf{p} - \not{e}A(t,\mathbf{x}))^2/(2m)$, which gives

$$(i\hbar\partial_t - e\phi(t,\mathbf{x}))\psi(t,\mathbf{x}) = \frac{1}{2m}(-i\hbar\nabla_{\mathbf{x}} - \not{e}A(t,\mathbf{x})))^2\psi(t,\mathbf{x}). \qquad (S)$$

The next crucial step of Schrödinger's theory is the identification of the stationary states with solutions of the type $\exp(-i\omega t)\psi(\mathbf{x})$ for the static Maxwell fields $\phi(t,\mathbf{x}) \equiv \phi(\mathbf{x})$ and $A(t,\mathbf{x}) \equiv A(\mathbf{x})$. This identification is suggested by the de Broglie plain wave $\exp(-i\omega t)\exp(i\mathbf{kx})$ where only the spatial factor has to be modified since the external field twists the space but not the time. The energy is again $E = \hbar\omega$. This identification leads to corresponding *stationary* equations (*eigenvalue* problems),

$$\frac{1}{c^2}(\omega - e\phi(\mathbf{x}))^2\psi(\mathbf{x}) = (-i\hbar\nabla_{\mathbf{x}} - \not{e}A(\mathbf{x}))^2\psi(\mathbf{x}) + m^2c^2\psi(\mathbf{x}), \qquad (KG_\omega)$$

$$(\omega - e\phi(\mathbf{x}))\psi(x) = \frac{1}{2m}(-i\hbar\nabla_{\mathbf{x}} - \not{e}A(\mathbf{x}))^2\psi(\mathbf{x}). \qquad (S_\omega)$$

for the determination of the energies $E = \hbar\omega$ and the amplitudes $\psi(\mathbf{x})$ of the stationary states.

Schrödinger has calculated all solutions to (S_ω) for the Hydrogen atom. The agreement with the experimentally observed spectrum was perfect. The calculation uses the standard separation of variables in spherical coordinates which involves some integer numbers as in the quantum conditions (D). Just this analogy suggested to Schrödinger an eigenvalue problem for the determination of the stationary states of the atom.

Nonrelativistic theory of Spin In 1925 Uhlenbeck and Goudsmit introduced the hypothesis of the existence of the *spin* of the electron, i.e. of its own magnetic and mechanical momentum with the gyromagnetic ratio $2r$, to explain the double-splitting of the spectral lines and the Einstein-de

Haas experiment. In 1927 Pauli obtained the wave equation which takes into account the spin of the electron,

$$(i\hbar\partial_t - e\phi(\mathbf{x}))\psi(t,\mathbf{x}) = \frac{1}{2m}(-i\hbar\nabla_{\mathbf{x}} - \not{A}(\mathbf{x}))^2\psi(t,\mathbf{x}) + \mu_B \sum_1^3 \sigma_k B_k(t,\mathbf{x})\psi(t,\mathbf{x}). \qquad (P)$$

Here $\mu_B = \dfrac{|e|\hbar}{2mc}$ is the *Bohr magneton*, the wave function $\psi(t,\mathbf{x}) = (\psi_1(t,\mathbf{x}), \psi_2(t,\mathbf{x}))$ with the complex-valued functions $\psi_k(t,\mathbf{x})$, B_k are the components of the magnetic field and σ_k are complex 2×2 *Pauli matrices*. Pauli obtained the equation by just postulating the double-splitting and covariance with respect to space rotations.

This equation describes the spin of the electron, i.e., it leads to the right gyromagnetic ratio observed in the Einstein-de Haas experiment. It also allowed Pauli to explain the (anomalous) Zeeman effect and the Stern-Gerlach experiment.

Relativistic theory of Spin In 1927 Dirac discovered the relativistic invariant equation which generalizes the Pauli and Klein-Gordon equations,

$$[\sum_{\alpha=0}^3 \gamma_\alpha(i\hbar\nabla_\alpha - \not{\mathcal{A}}_\alpha(x)) - m]\psi(x) = 0, \qquad x \in \mathbb{R}^4,$$

where $\nabla_0 = \partial_t/c$, $(\nabla_1,\nabla_2,\nabla_3) = \nabla_{\mathbf{x}}$, $\mathcal{A}_0(x) = \phi(x)$ and $\mathcal{A}_k = -A_k(x)$, $k = 1,2,3$, γ_α are the Dirac- 4×4-matrices, and $\psi(x) \in \mathbb{C}^4$ for $x \in \mathbb{R}^4$.

The Dirac equation also provides the right gyromagnetic ratio and explains the spin of the electron. It gives a much more exact description of the Hydrogen atom spectrum than the Schrodinger and Pauli equations.

Interference of the electrons In 1927 Davisson and Germer observed the interference of the electron beams. Later the experiments were repeated and confirmed by many authors: Thomson, Rupp, Kikouchi and others. In 1949 Biberman, Sushkin and Fabrikant observed the interference pattern with a weak beam with a very low rate of registration of the electrons.

The probabilistic interpretation of the wave function In 1927 Born proposed the following interpretation of the wave function to explain the Davisson-Germer experiment: $|\psi(t,\mathbf{x})|^2$ *is the Density of the Probability.*

1.2 On the contents of the lectures

The aim of these lectures is to give an introduction to Classical Field Theory and Quantum Mechanics for mathematicians. We explain carefully the tools which are necessary for the introduction:

i) The Lagrangian Theory for finite-dimensional dynamical systems, Noether Theorem I on the invariants in the presence of the symmetry, the Hamilton-Jacobi equation (Lectures 2-5).

ii) The Lagrangian Theory for the classical fields, a new simple and complete proof of the Noether Theorem II on the currents and its applications (Lectures 6-10).

iii) The Maxwell Theory in the Lagrangian form, the integral representations for the fields, the role of the *retarded potentals*, and the Hamiltonian equations for the charge in Maxwell Field (Lectures 11-14).

iv) The Lorentz theory of the Matter in Maxwell Field. We give a new rigorous introduction of the Magnetic Momentum of a molecule (Proposition 15.9) and the proof of the Macroscopic Limit in the sense of distributions (Lecture 15).

v) The Geometric Optics for free Schrödinger and Klein-Gordon Equations and the short-wave

WKB asymptotics for the Schrödinger Equation in a Maxwell field (Lecture 16).
vi) We explain all details of the calculations with spherical functions using Lie algebra of angular momentum (Lecture 18).
vii) Finally, we apply the Schrödinger Equation to the derivation of spectrum of the Hydrogen atom, dipole radiation and selection rules in a uniform magnetic field (Lectures 17 and 19-21).

Remarks i) The short-wave WKB asymptotics allows us to justify the introduction of the Schrödinger Equation as a matter equation suggested by the observation of the cathode rays. Let us note that J.J.Thomson's identification of the cathode rays with the beam of the electrons means that the rays are the solutions to the Lorentz Eqn (L) with an appropriate factor e/m. On the other hand, the rays arise in the short-wave WKB asymptotics of the solutions to Eqns (KG) and (S). Namely, the asymptotics have the form

$$\psi(t,\mathbf{x}) \sim a(t,\mathbf{x})\exp(\frac{i}{h}S(t,\mathbf{x})). \qquad (WKB)$$

The phase function $S(t,\mathbf{x})$ satisfies the Hamilton-Jacobi Eqn corresponding to the Lorentz Eqn (L). Therefore, $S(t,\mathbf{x})$ is given by an integral of the action along the trajectories of the Lorentz Eqn. Furthermore, the amplitude $a(t,\mathbf{x})$ satisfies the transport equations which means that, roughly speaking, the amplitude is the translation of the initial amplitude $a(x,0)$ along the trajectories of Eqn (L). This analysis suggests that the cathode rays are the short-wave solutions to the (KG) and (S) Equations.
ii) Thus the Schrödinger and Klein-Gordon Eqns "follow" directly from the particle-like behavior of the cathode rays and the Planck Law (P) which fix the small parameter $\hbar$. Let us note however that the introduction of the wave equations for the matter becomes necessary only after the Einstein explanation of the photoeffect, the Bohr analysis of the Ritz combination rule and the de Broglie's formulation of the wave-particle duality. The introduction of the *free* wave equations (KG_0), (S_0) in the de Broglie Theory is motivated by the algebraic arguments of relativistic invariance. Also the Schrödinger Eqns (KG), (S) formally follow from (KG_0), (S_0) by the algebraic arguments. More fundamental arguments rely on the central role of the action-function $S(t,\mathbf{x})$ which has been demonstrated by the Debye-Sommerfeld-Wilson Rule (D) in the "old" quantum theory. Note that the quantum conditions (D) appear also in the Schrödinger theory in the form of the Bohr-Sommerfeld relations, however with half-integer n.

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2 Newton Mechanics

2.1 One-particle

2.1.1 Newton equation

The motion of one particle of the mass $m > 0$ is governed by the Newton differential equation

$$m\ddot{\mathbf{q}}(t) = F(\mathbf{q}(t), t), \quad t \in \mathbb{R}. \tag{2.1}$$

Here $\mathbf{q}(t) \in \mathbb{R}^3$ is the particle position at time t and $F(\cdot)$ is the force field. Let us assume that $F \in C^1(\mathbb{R}^3 \times \mathbb{R}, \mathbb{R}^3)$. Then the solution $\mathbf{q}(t)$ is defined uniquely by the initial conditions $\mathbf{q}(0) = \mathbf{q}_0 \in \mathbb{R}^3$, $\dot{\mathbf{q}}(0) = \mathbf{v}_0 \in \mathbb{R}^3$ by the Main Theorem of Ordinary Differential Equations. The solution exists for $|t| \le \varepsilon$, where $\varepsilon > 0$ depends on initial data $\mathbf{q}_0, v_0$.

2.1.2 Energy conservation

Let us assume that the force field F has a *potential function* (or simply *potential*) $V(\cdot) \in C^2(\mathbb{R}^3 \times \mathbb{R})$,

$$F(\mathbf{q}, t) = -\nabla V(\mathbf{q}, t), \quad \mathbf{q} \in \mathbb{R}^3, \quad t \in \mathbb{R}. \tag{2.2}$$

Definition 2.1 *i)* $\mathcal{E} := \mathbb{R}^3 \times \mathbb{R}^3$ *is the* **phase space** *of the Newton equation,* $\mathcal{E}^+ := \mathbb{R}^3 \times \mathbb{R}^3 \times \mathbb{R}$ *is the* **extended phase space** *of the Newton equation,*
ii) Energy $E(\mathbf{q}, \mathbf{v}, t)$ *is the function on the extended phase space,*

$$E(\mathbf{q}, \mathbf{v}, t) = \frac{m\mathbf{v}^2}{2} + V(\mathbf{q}, t), \quad (\mathbf{q}, \mathbf{v}, t) \in \mathcal{E}^+. \tag{2.3}$$

Theorem 2.2 *Let the condition (2.2) hold and the potential does not depend on t,*

$$V(\mathbf{q}, t) \equiv V(\mathbf{q}), \quad (\mathbf{q}, t) \in \mathbb{R}^3 \times \mathbb{R}. \tag{2.4}$$

Then for every solution $\mathbf{q}(t) \in C^2([t_0, t_1], \mathbb{R}^3)$ *to the Newton equation, the energy is conserved,*

$$E(t) := E(\mathbf{q}(t), \dot{\mathbf{q}}(t)) = \text{const}, \quad t \in [t_0, t_1]. \tag{2.5}$$

Proof By the chain rule of the differentiation, the Newton equation (2.1) and (2.2),

$$\dot{E}(t) = m\dot{\mathbf{q}}(t) \cdot \ddot{\mathbf{q}}(t) + \nabla V(\mathbf{q}(t)) \cdot \dot{\mathbf{q}}(t) = [m\ddot{\mathbf{q}}(t) + \nabla V(\mathbf{q}(t))] \cdot \dot{\mathbf{q}}(t) = 0, \quad t \in [t_0, t_1]. \tag{2.6}$$

2.1.3 Well-posedness condition

Theorem 2.3 *Let the condition (2.4) hold and the potential is bounded from below, by some constant* $C \in \mathbb{R}$*:*

$$V(\mathbf{q}) \ge C, \quad \mathbf{q} \in \mathbb{R}^3. \tag{2.7}$$

Then every solution $\mathbf{q}(t)$ *to the Newton equation (2.1) exists globally in time, i.e. for all* $t \in \mathbb{R}$.

Proof The energy conservation (2.5) implies that the velocity is bounded, $|\dot{\mathbf{q}}(t)| \le$const. Then also $\mathbf{q}(t)$ is bounded. This provides the existence of the global solution for all $t \in \mathbb{R}$. ■

2.2 Many particles

2.2.1 Newton equations

The motion of n particles of the masses $m_i > 0$ is governed by the Newton differential equation

$$m_i \ddot{\mathbf{q}}_i(t) = F_i(q(t), t), \ t \in \mathbb{R}, \quad i = 1, ..., n. \tag{2.8}$$

Here
i) $\mathbf{q}_i(t) \in \mathbb{R}^3$ is the position of the i-th particle at time t, $q(t) = (\mathbf{q}_1(t), ..., \mathbf{q}_n(t)) \in \mathbb{R}^{3n}$ and
ii) $F_i(q(t), t) \in \mathbb{R}^3$ is the force acting on the i-th particle.

Let us assume that the force field $F(q,t) := (F_1(q,t), ..., F_n(q,t)) \in C^1(\mathbb{R}^{3n} \times \mathbb{R}, \mathbb{R}^{3n})$. Then the solution $q(t) = (\mathbf{q}_1(t), ..., \mathbf{q}_n(t))$ to the system (2.8) is defined uniquely by the initial conditions $q(0) = q_0 \in \mathbb{R}^{3n}$, $\dot{q}(0) = v_0 \in \mathbb{R}^{3n}$ by the Main Theorem of Ordinary Differential Equations. The solution exists for $|t| \le \varepsilon$, where $\varepsilon > 0$ depends on initial data $q_0, \mathbf{v}_0$.

2.2.2 Energy conservation

Let us assume that the force fiel4 F has a *potential function* (or simply *potential*) $V(\cdot) \in C^2(\mathbb{R}^{3n})$,

$$F_i(q,t) = -\nabla_{\mathbf{q}_i} V(q,t), \quad q \in \mathbb{R}^{3n}, \ \ i = 1, ..., n. \tag{2.9}$$

Definition 2.4 *i)* $\mathcal{E} = \mathbb{R}^{3n} \times \mathbb{R}^{3n}$ *is the* **phase space** *of the Newton system (2.8),* $\mathcal{E}^+ := \mathbb{R}^{3n} \times \mathbb{R}^{3n} \times \mathbb{R}$ *is the* **extended phase space** *of the Newton system (2.8).*
ii) Energy $E(q, v, t)$ *is the function on the phase space,*

$$E(q, v, t) = \sum_i \frac{m_i \mathbf{v}_i^2}{2} + V(q,t), \quad (q, v) \in \mathcal{E}, \tag{2.10}$$

where $v = (\mathbf{v}_1, ..., \mathbf{v}_n)$.

Let us call *the trajectory* any solution $q(t)$ to the Newton system (2.8)

Theorem 2.5 *Let the condition (2.9) hold and the potential does not depend on t,*

$$V(q,t) \equiv V(q), \quad (q,t) \in \mathbb{R}^{3n} \times \mathbb{R}. \tag{2.11}$$

Then for any trajectory $q(t) \in C^2([t_0, t_1], \mathbb{R}^{3n})$*, the energy is conserved,*

$$E(t) := E(q(t), \dot{q}(t)) = \text{const}, \ \ t \in [t_0, t_1]. \tag{2.12}$$

Proof By the chain rule of the differentiation, the Newton system (2.8) and (2.9) imply,

$$\begin{aligned} \dot{E}(t) &= \sum_i m_i \dot{\mathbf{q}}_i(t) \cdot \ddot{\mathbf{q}}_i(t) + \sum_i \nabla_{\mathbf{q}_i} V(q(t)) \cdot \dot{\mathbf{q}}_i(t) \\ &= \sum_i [m_i \ddot{\mathbf{q}}_i(t) + \nabla_{\mathbf{q}_i} V(q(t))] \cdot \dot{\mathbf{q}}_i(t) = 0, \qquad t \in [t_0, t_1]. \end{aligned} \tag{2.13}$$

2.2.3 Well-posedness condition

Theorem 2.6 *Let the condition (2.11) hold and the potential is bounded from below, by some constant* $C \in \mathbb{R}$*:*

$$V(q) \ge C, \quad q \in \mathbb{R}^{3n}. \tag{2.14}$$

Then every solution $q(t)$ *to the Newton equation (2.8) exists globally in time, i.e. for all* $t \in \mathbb{R}$.

Proof The energy conservation (2.12) implies that the velocity is bounded, $|\dot{q}(t)| \le$const. Then also $q(t)$ is bounded. This provides the existence of the global solution for all $t \in \mathbb{R}$. ■

2.3 Symmetry theory

The invariance of the potential V with respect to the translation in time, (2.11), provides the energy conservation (2.12). Let us show that the invariance of the potential $V(q)$ with respect to some transformation of the *configuration space* $Q := \mathbb{R}^{3n}$ leads to new conservation laws.

2.3.1 Translation group

Let us fix a vector $h \neq 0$ in $\mathbb{R}^3$ and consider the translations $x \mapsto x + hs$ of $\mathbb{R}^3$ and corresponding action in $\mathbb{R}^{3n}$:

$$T_s(\mathbf{q}_1, , , ., \mathbf{q}_n) = (\mathbf{q}_1 + hs, , , ., \mathbf{q}_n + hs), \quad (\mathbf{q}_1, , , ., \mathbf{q}_n) \in \mathbb{R}^{3n}. \tag{2.15}$$

Definition 2.7 *The system (2.8) is invariant with respect to the translations (2.15) if*

$$V(T_s(q), t) = V(q, t), \quad (q, t) \in \mathbb{R}^{3n+1}, \quad \forall s \in \mathbb{R}. \tag{2.16}$$

Example 2.8 *The Newton system (2.8) is invariant with respect to the translations (2.15) with every $h \in \mathbb{R}^3$, if the potential energy has the structure*

$$V(\mathbf{q}_1, ..., \mathbf{q}_n, t) = W(\mathbf{q}_1 - \mathbf{q}_n, ..., \mathbf{q}_{n-1} - \mathbf{q}_n, t), \quad (\mathbf{q}_1, ..., \mathbf{q}_n, t) \in \mathbb{R}^{3n+1} \tag{2.17}$$

with a function W of $3n-1$ variables.

Definition 2.9 *i) The momentum p_i of the i-th particle is the vector-function on the phase space $\mathcal{E}$,*

$$p_i := m_i \mathbf{v}_i \in \mathbb{R}^3, \quad (q, v) \in \mathcal{E}. \tag{2.18}$$

ii) the (total) momentum p of the system (2.8) is the vector-function on the phase space $\mathcal{E}$,

$$p := \sum_i p_i = \sum_i m_i \mathbf{v}_i \in \mathbb{R}^3, \quad (q, v) \in \mathcal{E}. \tag{2.19}$$

iii) Center of mass of the system of n particles

$$Q := \frac{1}{M} \sum_i m_i \mathbf{q}_i, \quad q = (\mathbf{q}_1, ..., \mathbf{q}_n) \in \mathbb{R}^{3n}, \tag{2.20}$$

where $M := \sum_i m_i$ is the total mass of the system.

Theorem 2.10 *Let (2.9) hold and the system (2.8) be invariant with respect to the translations (2.15) along a fixed vector $h \in \mathbb{R}^3$. Then for any trajectory $q(t) \in C^2([t_0, t_1], \mathbb{R}^{3n})$, the projection of the momentum $p(t)$ onto h is conserved,*

$$p_h(t) := p(t) \cdot h = \text{const}, \quad t \in [t_0, t_1]. \tag{2.21}$$

Proof By (2.9), the system (2.8) and the chain rule of the differentiation,

$$\dot{p}_h(t) = \sum_i m_i \ddot{\mathbf{q}}_i(t) \cdot h = -\sum_i \nabla_{\mathbf{q}_i} V(q(t), t) \cdot h = -\frac{d}{ds}\bigg|_{s=0} V(T_s q(t), t) = 0, \quad t \in [t_0, t_1] \tag{2.22}$$

by (2.16). ■

Corollary 2.11 *Let the Newton system (2.8) be invariant with respect to the translations (2.15) along all vectors $h \in \mathbb{R}^3$. Then for any trajectory, the momentum $p(t)$ is conserved, $p(t) = \text{const}$, and the center of mass $Q(t) = \sum_i m_i \mathbf{q}_i(t)/M$ moves uniformly: $Q(t) = \mathbf{v}t + Q_0$.*

Proof Since (2.22) holds for every h, we have $p(t) = \text{const}$ and

$$\ddot{Q}(t) = \frac{1}{M}\sum_i m_i \ddot{\mathbf{q}}_i = 0. \qquad \blacksquare$$

2.3.2 Rotation group

Let us fix a unit vector $r \in \mathbb{R}^3$ and consider the rotation round r in $\mathbb{R}^3$ with angle s *radian*. Let us denote by $O_r(s) \in SO(3)$ the corresponding orthogonal matrix and define corresponding transformation in $\mathbb{R}^{3n}$ by

$$R_s(\mathbf{q}_1, ..., \mathbf{q}_n) = (O_r(s)\mathbf{q}_1, ..., O_r(s)\mathbf{q}_n), \quad (\mathbf{q}_1, ..., \mathbf{q}_n) \in \mathbb{R}^{3n}. \tag{2.23}$$

Definition 2.12 *The system (2.8) is invariant with respect to the rotations (2.23) if*

$$V(R_s(q), t) = V(q, t), \quad (q, t) \in \mathbb{R}^{3n+1}, \quad \forall s \in \mathbb{R}. \tag{2.24}$$

Example 2.13 *The system (2.8) is invariant with respect to the rotations (2.15) with every $r \in \mathbb{R}^3$, if the potential energy has the structure*

$$V(\mathbf{q}_1, ..., \mathbf{q}_n, t) = W(\{|\mathbf{q}_i - \mathbf{q}_j| : 1 \le i < j \le n\}, t), \quad (\mathbf{q}_1, ..., \mathbf{q}_n, t) \in \mathbb{R}^{3n+1}. \tag{2.25}$$

Definition 2.14 *i) The angular momentum M_i of the i-th particle is the vector-function on the phase space $\mathcal{E}$,*

$$M_i(q, v) := \mathbf{q}_i \times p_i \in \mathbb{R}^3, \quad (q, v) \in \mathcal{E}. \tag{2.26}$$

ii) the angular momentum M of the Newton system (2.8) is the vector-function on the phase space $\mathcal{E}$,

$$M(q, v) := \sum_i M_i = \sum_i \mathbf{q}_i \times p_i \in \mathbb{R}^3, \quad (q, v) \in \mathcal{E}. \tag{2.27}$$

Theorem 2.15 *Let the Newton system (2.8) be invariant with respect to the rotations (2.23) round a fixed vector $r \in \mathbb{R}^3$. Then for any trajectory $q(t) \in C^2([t_0, t_1], \mathbb{R}^{3n})$, the projection of the angular momentum $M(q(t), \dot{q}(t))$ onto r is conserved,*

$$M_r(t) := M(q(t), \dot{q}(t)) \cdot r = \text{const}, \quad t \in [t_0, t_1]. \tag{2.28}$$

Proof The differentiation gives,

$$\begin{aligned} \dot{M}_r(t) &= [\sum_i \dot{\mathbf{q}}_i(t) \times p_i(t) + \sum_i \mathbf{q}_i(t) \times \dot{p}_i(t)] \cdot r \\ &= [\sum_i \dot{\mathbf{q}}_i(t) \times m_i \dot{\mathbf{q}}_i(t) + \sum_i \mathbf{q}_i(t) \times m_i \ddot{\mathbf{q}}_i(t)] \cdot r \\ &= \sum_i [\mathbf{q}_i(t) \times m_i \ddot{\mathbf{q}}_i(t)] \cdot r = \sum_i m_i \ddot{\mathbf{q}}_i(t) \cdot [r \times \mathbf{q}_i(t)]. \end{aligned} \tag{2.29}$$

Therefore, the Newton system (2.8) and (2.27) imply by the chain rule of the differentiation,

$$\dot{M}_r(t) = -\sum_i \nabla_{\mathbf{q}_i} V(q(t), t) \cdot [r \times \mathbf{q}_i(t)] = -\frac{d}{ds}\Big|_{s=0} V(R_s q(t), t) = 0, \quad t \in [t_0, t_1]. \tag{2.30}$$

by (2.24) since

$$r \times \mathbf{q}_i(t) = \left.\frac{d}{ds}\right|_{s=0} O_r(s)\mathbf{q}_i(t). \tag{2.31}$$

This identity follows from the fact that the vectors in both sides are orthogonal to the plane containing r and $\mathbf{q}_i(t)$, and have the same length. Indeed, the length of the LHS is $|r|\,|\mathbf{q}_i(t)|\sin\alpha$, where α is the angle between r and $\mathbf{q}_i(t)$, and the length of the RHS is the radius of the circle $\{O_r(s)\mathbf{q}_i(t) : s \in [0, 2\pi]\}$ which is equal to $|\mathbf{q}_i(t)|\sin\alpha$. ■

3 Lagrangian Mechanics

3.1 One particle

3.1.1 Lagrangian function

We expose the Lagrangian variational form of the Newton Eqn (2.1) with the potential (2.2),

$$m\ddot{\mathbf{q}}(t) = -\nabla V(\mathbf{q}(t), t), \quad t \in \mathbb{R}. \tag{3.1}$$

Definition 3.1 *Lagrangian $L(\mathbf{q}, \mathbf{v}, t)$ of the system is the function on the extended phase space $\mathcal{E}^+ = \mathbb{R}^3 \times \mathbb{R}^3 \times \mathbb{R}$ defined by (cf. (2.3)),*

$$L(\mathbf{q}, \mathbf{v}, t) = \frac{m\mathbf{v}^2}{2} - V(\mathbf{q}, t), \quad (\mathbf{q}, \mathbf{v}, t) \in \mathcal{E}^+. \tag{3.2}$$

Exercise 3.2 *Check that the Newton equation (3.1) can be represented in the* **Euler-Lagrange** *form,*

$$\frac{d}{dt} L_{\mathbf{v}}(\mathbf{q}(t), \dot{\mathbf{q}}(t), t) = L_{\mathbf{q}}(\mathbf{q}(t), \dot{\mathbf{q}}(t), t), \quad t \in \mathbb{R}. \tag{3.3}$$

Let us consider more general Lagrangian systems with an arbitrary function $L(\mathbf{q}, \mathbf{v}, t)$.

Definition 3.3 *i) The Lagrangian system with one particle is the dynamical system described by the Lagrangian equation (3.3) with a function $L(\mathbf{q}, \mathbf{v}, t) \in C^2(\mathcal{E}^+)$.*
ii) The momentum of the Lagrangian system is the vector-function on the extended phase space $\mathcal{E}^+$ defined by

$$\mathbf{p} = L_{\mathbf{v}}(\mathbf{q}, \mathbf{v}, t), \quad (\mathbf{q}, \mathbf{v}, t) \in \mathcal{E}^+. \tag{3.4}$$

iii) The energy of the Lagrangian system is the function on the extended phase space $\mathcal{E}^+$ defined by

$$E(\mathbf{q}, \mathbf{v}, t) = \mathbf{pv} - L(\mathbf{q}, \mathbf{v}, t), \quad (\mathbf{q}, \mathbf{v}, t) \in \mathcal{E}^+. \tag{3.5}$$

Example 3.4 *The Newton equation (3.1) is the Lagrangian system with the Lagrangian functional (3.2), momentum $\mathbf{p} = m\mathbf{v}$ and the energy $E = \dfrac{m\mathbf{v}^2}{2} + V(\mathbf{q}, t)$*

Theorem 3.5 *Let the Lagrangian do not depend on time,*

$$L(\mathbf{q}, \mathbf{v}, t) = L(\mathbf{q}, \mathbf{v}), \quad (\mathbf{q}, \mathbf{v}, t) \in \mathcal{E}^+. \tag{3.6}$$

Then for any trajectory $\mathbf{q}(t) \in C^2([t_0, t_1], \mathbb{R}^3)$, the energy is conserved, (2.5).

Proof The differentiation of (3.5) with $\mathbf{q} = \mathbf{q}(t)$ and $\mathbf{v} = \dot{\mathbf{q}}(t)$ gives,

$$\dot{E}(t) = \dot{\mathbf{p}}\mathbf{v} + \mathbf{p}\dot{\mathbf{v}} - L_{\mathbf{q}}\dot{\mathbf{q}} - L_{\mathbf{v}}\dot{\mathbf{v}} = 0 \tag{3.7}$$

by the equations (3.3) and the definition (3.4). ■

Exercise 3.6 *Calculate the momentum and the energy for the Lagrangian $L(\mathbf{q}, \mathbf{v}) = -m\sqrt{1 - \mathbf{v}^2}$.*

3.1.2 Action functional

Definition 3.7 *$C^1 = C^1([0,\infty), \mathbb{R}^3)$ is the space of all paths in the 3D space.*

We will consider the real-valued functionals $\mathcal{F}$ on C^1. By definition, $\mathcal{F}$ is a map $C^1 \to \mathbb{R}$.

Example 3.8 $\mathcal{F}(\mathbf{q}) = \int_0^T |\dot{\mathbf{q}}(t)|dt$ *is the length of the path* $\mathbf{q}(\cdot) \in C^1$, $t \in [0,T]$.

Definition 3.9 *The Gateau differential $D\mathcal{F}(\mathbf{q})$ is the* **linear** *functional $C^1 \mapsto \mathbb{R}$ defined by*

$$\langle D\mathcal{F}(\mathbf{q}), h\rangle = \frac{d}{d\varepsilon}\bigg|_{\varepsilon=0} \mathcal{F}(\mathbf{q}+\varepsilon h), \quad h(\cdot) \in C^1 \tag{3.8}$$

if the derivative in the RHS exists.

Let us fix a $T > 0$.

Definition 3.10 *The action is the functional on C^1 defined by*

$$S_T(\mathbf{q}(\cdot)) = \int_0^T L(\mathbf{q}(t), \dot{\mathbf{q}}(t), t)dt, \quad \mathbf{q}(\cdot) \in C^1. \tag{3.9}$$

Note that the functional is defined on the whole of C^1 if $L(\mathbf{q},\mathbf{v},t) \in C(\mathcal{E}^+)$. Moreover, the functional is differentiable if $L(\mathbf{q},\mathbf{v},t) \in C^1(\mathcal{E}^+)$:

Lemma 3.11 *The Gateau differential $DS_T(\mathbf{q})$ exists for $\mathbf{q} \in C^1$.*

Proof From definition 3.9 we get by the theorem of the differentiation of integrals,

$$\begin{aligned} \langle DS_T(\mathbf{q}), h\rangle : &= \frac{d}{d\varepsilon}\bigg|_{\varepsilon=0} \int_0^T L(\mathbf{q}(t)+\varepsilon h(t), \dot{\mathbf{q}}(t)+\varepsilon\dot{h}(t), t)dt \\ &= \int_0^T [L_{\mathbf{q}}(\mathbf{q}(t),\dot{\mathbf{q}}(t))h(t) + L_{\mathbf{v}}(\mathbf{q}(t),\dot{\mathbf{q}}(t),t)\dot{h}(t)]dt \end{aligned} \tag{3.10}$$

since $L(\mathbf{q},\mathbf{v},t) \in C^2(\mathcal{E}^+)$ by our basic assumptions. ■

3.1.3 The Hamilton Least Action Principle

Let us introduce the space of *variations*.

Definition 3.12 $C^1(T) = \{h \in C^1 : h(0) = h(T) = 0\}$.

Definition 3.13 *The function $\mathbf{q} \in C^1$ satisfies the Hamilton Least Action Principle (LAP) if for any $T > 0$,*

$$\langle DS_T(\mathbf{q}), h\rangle = 0, \quad \forall h(\cdot) \in C^1(T) \tag{3.11}$$

Theorem 3.14 *For $\mathbf{q} \in C^2([0,\infty), \mathbb{R}^3)$ the Hamilton LAP is equivalent to the Euler-Lagrange Eqns (3.3) with $t \in [0,T]$.*

Proof The partial integration in (3.10) gives,

$$\langle DS_T(\mathbf{q}), h\rangle = \int_0^T [L_{\mathbf{q}}(\mathbf{q}(t), \dot{\mathbf{q}}(t), t) - \frac{d}{dt} L_{\mathbf{v}}(\mathbf{q}(t), \dot{\mathbf{q}}(t), t)] h(t) dt, \quad h \in C_0^1(T). \tag{3.12}$$

Therefore, (3.11) is equivalent to (3.3) by the following lemma:

Lemma 3.15 Main Lemma of the Calculus of Variations *(du Bois-Reymond).*
Let a function $f(t) \in C[0,T]$ and $\int_0^T f(t)h(t)dt = 0$ for any function $h(t) \in C[0,T]$ with the boundary values $h(0) = h(T) = 0$. Then $f(t) = 0$, $t \in [0,T]$.

Exercise 3.16 *To prove the Main Lemma.*

3.2 n particles

3.2.1 Lagrangian function

We extend the Lagrangian formalism to the Newton Eqns (2.8) with the potential (2.9),

$$m_i \ddot{\mathbf{q}}_i(t) = -\nabla_{\mathbf{q}_i} V(q(t), t), \quad t \in \mathbb{R}. \tag{3.13}$$

Let us introduce the Lagrangian $L(q, v, t)$ of the system (3.13) as the function on the extended phase space $\mathcal{E}^+ = \mathbb{R}^{3n} \times \mathbb{R}^{3n} \times \mathbb{R}$ defined by (cf. (3.2)),

$$L(q, v, t) = \sum_i \frac{m_i \mathbf{v}_i^2}{2} - V(q, t), \quad (q, v, t) \in \mathcal{E}^+, \tag{3.14}$$

where $v = (\mathbf{v}_1, ...\mathbf{v}_n)$.

Exercise 3.17 *Check that the Newton equation (3.13) can be represented in the* **Euler-Lagrange** *form,*

$$\frac{d}{dt} L_v(q(t), \dot{q}(t), t) = L_q(q(t), \dot{q}(t), t), \quad t \in \mathbb{R}. \tag{3.15}$$

Let us consider more general Lagrangian systems with the extended phase space $\mathcal{E}^+ := \mathbb{R}^N \times \mathbb{R}^N \times \mathbb{R}$, where $N = 1, 2...$, and an arbitrary function $L(q, v, t)$.

Definition 3.18 *i) The Lagrangian system in the extended phase space $\mathcal{E}^+ := \mathbb{R}^N \times \mathbb{R}^N \times \mathbb{R}$ is the dynamical system described by the equations (3.15) with a function $L(q, v, t) \in C^2(\mathcal{E})$.*
ii) The momentum of the Lagrangian system is the vector-function on the extended phase space $\mathcal{E}^+$ defined by

$$p = L_v(q, v, t), \quad (q, v, t) \in \mathcal{E}^+. \tag{3.16}$$

iii) The energy of the Lagrangian system is the function on the phase space $\mathcal{E}^+$ defined by

$$E(q, v, t) = pv - L(q, v, t), \quad (q, v, t) \in \mathcal{E}^+. \tag{3.17}$$

Exercise 3.19 *Check that the Newton equations (3.13) are the Lagrangian system with the Lagrangian functional (3.14), momentum $p = (\mathbf{p}_1, ..., \mathbf{p}_n)$ where $\mathbf{p}_i = m_i \mathbf{v}_i$, and the energy*

$$E = \sum_i \frac{m_i \mathbf{v}_i^2}{2} + V(q, t). \tag{3.18}$$

Theorem 3.20 *Let the Lagrangian do not depend on time,*

$$L(q,v,t) = L(q,v), \quad (q,v,t) \in \mathcal{E}^+. \tag{3.19}$$

Then for any trajectory $q(t) \in C^2([t_0,t_1],\mathbb{R}^N)$, the energy is conserved, (2.12).

Proof The differentiation of (3.17) with $q = q(t)$ and $v = \dot{q}(t)$ gives,

$$\dot{E}(t) = \dot{p}v + p\dot{v} - L_q\dot{q} - L_v\dot{v} = 0 \tag{3.20}$$

by the equations (3.15) and the definition (3.16). ■

3.2.2 Action functional

Definition 3.21 *$C^1 = C^1([0,\infty),\mathbb{R}^N)$ is the space of all paths in the ND space.*

We will consider the real-valued functionals $\mathcal{F}$ on C^1. By definition, $\mathcal{F}$ is a map $C^1 \to \mathbb{R}$.

Example 3.22 $\mathcal{F}(q) = \int_0^T |\dot{q}(t)|dt$ *is the length of the path $q(\cdot) \in C^1$, $t \in [0,T]$.*

Definition 3.23 *The Gateau differential $D\mathcal{F}(q)$ is the* **linear** *functional $C^1 \mapsto \mathbb{R}$ defined by*

$$\langle D\mathcal{F}(q), h\rangle = \left.\frac{d}{d\varepsilon}\right|_{\varepsilon=0} \mathcal{F}(q+\varepsilon h) \tag{3.21}$$

for $h(\cdot) \in C^1$ if the derivative in the RHS exists.

Let us fix a $T > 0$.

Definition 3.24 *The action is the functional on $C^1(T)$ defined by*

$$S_T(q) = \int_0^T L(q(t),\dot{q}(t))dt, \quad q(\cdot) \in C^1. \tag{3.22}$$

Note that the functional is defined on the whole of $C^1(T)$ if $L(q,v) \in C(\mathcal{E})$. Moreover, the functional is differentiable if $L(q,v) \in C^1(\mathcal{E})$:

Lemma 3.25 *The Gateau differential $DS_T(q)$ exists for $q(\cdot) \in C^1$.*

Proof From definition 3.9 we get by the theorem of the differentiation of the integrals,

$$\begin{aligned} \langle DS_T(q), h\rangle : &= \left.\frac{d}{d\varepsilon}\right|_{\varepsilon=0} \int_0^T L(q(t)+\varepsilon h(t), \dot{q}(t)+\varepsilon\dot{h}(t))dt \\ &= \int_0^T [L_q(q(t),\dot{q}(t))h(t) + L_v(q(t),\dot{q}(t))\dot{h}(t)]dt \end{aligned} \tag{3.23}$$

since $L(q,v) \in C^2(\mathcal{E})$ by our basic assumptions. ■

3.2.3 The Hamilton Least Action Principle

Let us introduce the space of *variations*.

Definition 3.26 $C^1(T) = \{h(\cdot) \in C^1 : h(0) = h(T) = 0\}$.

Definition 3.27 *The function $q \in C^1$ satisfies the Hamilton Least Action Principle (LAP) if for any $T > 0$*

$$\langle DS_T(q), h\rangle = 0, \quad \forall h(\cdot) \in C^1(T) \tag{3.24}$$

Theorem 3.28 *For $q \in C^2([0,\infty), \mathbb{R}^N)$ the Hamilton LAP is equivalent to the Euler-Lagrange Eqns (3.15).*

Proof The partial integration in (3.23) gives,

$$\langle DS(q), h\rangle = \int_0^T [L_q(q(t), \dot q(t)) - \frac{d}{dt} L_v(q(t), \dot q(t))]h(t)dt. \tag{3.25}$$

Therefore, (3.24) is equivalent to (3.15) by the Main Lemma of the Calculus of Variations. ■

Remark 3.29 *The expositions in Sections 3.1 and 3.2 formally are almost identical.*

4 E.Noether Theory of Invariants

The invariance of the Lagrangian L with respect to the translation in time, (3.19), provides the energy conservation (2.5). Let us show that the invariance of the Lagrangian with respect to some transformation of the *configuration space* $Q := \mathbb{R}^N$ leads to new conservation laws.

4.1 Symmetry and Noether Theorem I

Consider a group $G = \{g\}$ of differentiable transformations $g \in C^2(Q, Q)$ of the configuration space Q of a Lagrangian system.

Definition 4.1 *G is a* **symmetry group** *of the Lagrangian system if the identity holds*

$$L(g(q), dg(q)v, t) = L(q, v, t), \ (q, v, t) \in \mathcal{E}^+, \quad \forall g \in G, \tag{4.1}$$

where $dg : \mathbb{R}^N \to \mathbb{R}^N$ is the differential of g.

Let us recall the definition of the differential:

$$dg(q)v := \left.\frac{dg(Q(\tau))}{d\tau}\right|_{\tau=0} \tag{4.2}$$

if $Q(0) = q$ and $\dot{Q}(0) = v$.

Consider a **one-parametric subgroup** $\{g_s \in G : s \in \mathbb{R}\}$ of the symmetry group G,

$$L(g_s(q), dg_s(v), t) = L(q, v, t), \ (q, v, t) \in \mathcal{E}^+, \quad \forall s \in \mathbb{R}. \tag{4.3}$$

Remark 4.2 *Since g_s is the one-parametric subgroup, we have $g_0 = Id$, hence*

$$(g_0(q), dg_0(v)) = (q, v), \qquad (q, v) \in \mathcal{E}. \tag{4.4}$$

Definition 4.3 *The Noether invariant is the function on the extended phase space $\mathcal{E}^+$ defined by*

$$I(q, v, t) = L_v(q, v, t)\left.\frac{dg_s(q)}{ds}\right|_{s=0}, \quad (q, v, t) \in \mathcal{E}^+. \tag{4.5}$$

Theorem 4.4 *(E.Noether [11]) Let $q(t) \in C^2(\mathbb{R}, \mathbb{R}^N)$ be a solution to the Euler-Lagrange Eqns (3.15) and $\{g_s : s \in \mathbb{R}\}$ the a one-parametric symmetry group of the Lagrangian system. Then $I(t) := I(q(t), \dot{q}(t), t) =$const, $t \in \mathbb{R}$.*

Proof Differentiation gives,

$$\dot{I}(t) = \frac{d}{dt}L_v(q(t), \dot{q}(t), t) \left.\frac{d}{ds}\right|_{s=0} g_s(q(t)) + L_v(q(t), \dot{q}(t), t) \left.\frac{d}{dt}\frac{d}{ds}\right|_{s=0} g_s(q(t)). \tag{4.6}$$

For the first summand on the RHS the Eqns (3.15) give,

$$\frac{d}{dt}L_v(q(t), \dot{q}(t), t) \left.\frac{d}{ds}\right|_{s=0} g_s(q(t)) = L_q(q(t), \dot{q}(t), t) \left.\frac{d}{ds}\right|_{s=0} g_s(q(t)). \tag{4.7}$$

For the second summand we have

$$L_v(q(t),\dot q(t),t)\ \frac{d}{dt}\frac{d}{ds}\Big|_{s=0} g_s(q(t)) = L_v(q(t),\dot q(t),t)\ \frac{d}{ds}\Big|_{s=0}\frac{d}{dt}g_s(q(t)) \tag{4.8}$$

by the well known identity $\dfrac{\partial^2}{\partial t\partial s} = \dfrac{\partial^2}{\partial s\partial t}$. At last,

$$\frac{d}{dt}g_s(q(t)) = dg_s(q(t))\dot q(t) \tag{4.9}$$

by definition (4.2) of the differential of the map g_s. Now (4.6)-(4.9) gives by the chain rule and (4.4),

$$\begin{aligned}\dot I(t) &= L_q(q(t),\dot q(t),t)\frac{d}{ds}\Big|_{s=0} g_s(q(t)) + L_v(q(t),\dot q(t),t)\frac{d}{ds}\Big|_{s=0} dg_s(q(t))\dot q(t)\\ &= \frac{d}{ds}\Big|_{s=0} L(g_s(q(t)), dg_s(q(t))\dot q(t),t) = 0 \qquad (4.10)\end{aligned}$$

according to (4.1). ■

4.2 Applications to n-particle systems

Let us apply the Noether Theorem to the Lagrangian systems of n particles i.e. with $N = 3n$ and $q = (\mathbf{q}_1, ..., \mathbf{q}_n)$ where $\mathbf{q}_i \in \mathbb{R}^3$.

4.2.1 Translation group

Let us fix a vector $h \neq 0$ in $\mathbb{R}^3$ and consider the transformation T_s from (2.15). By Definition 4.1 the Lagrangian system is invariant with respect to the translations (2.15) if

$$L(T_s(q), dT_s(q)v, t) = L(q,v,t),\ \ (q,v,t)\in\mathcal{E}^+,\quad \forall s\in\mathbb{R}. \tag{4.11}$$

Exercise 4.5 *Check that for the translations T_s, $s \in \mathbb{R}$, the differential is given by*

$$dT_s(q)v = v,\quad q, v \in \mathbb{R}^{3n}. \tag{4.12}$$

Exercise 4.6 *Check that the Lagrangian system is invariant with respect to the translations (2.15) with every $h \in \mathbb{R}^3$, if the Lagrangian has the structure (cf. (2.17)),*

$$L(\mathbf{q}_1, ..., \mathbf{q}_n, v, t) = \Lambda(\mathbf{q}_1 - \mathbf{q}_n, ..., \mathbf{q}_{n-1} - \mathbf{q}_n, v, t),\quad (\mathbf{q}_1, ..., \mathbf{q}_n, v, t)\in\mathcal{E}^+. \tag{4.13}$$

Definition 4.7 *i) The momentum p_i of the i-th particle of the Lagrangian system is the vector-function on the space $\mathcal{E}^+$,*

$$\mathbf{p}_i(q,v,t) := L_{\mathbf{v}_i}(q,v,t)\in\mathbb{R}^3,\quad (q,v,t)\in\mathcal{E}^+. \tag{4.14}$$

ii) the momentum p of the Lagrangian system is the vector-function on the space $\mathcal{E}^+$,

$$p(q,v,t) := \sum_i \mathbf{p}_i = \sum_i L_{\mathbf{v}_i}\in\mathbb{R}^3,\quad (q,v,t)\in\mathcal{E}^+. \tag{4.15}$$

Theorem 4.8 *Let the Lagrangian system (2.8) be invariant with respect to the translations (2.15) along a fixed vector $h \in \mathbb{R}^3$. Then for any trajectory $q(t) \in C^2([t_0,t_1],\mathbb{R}^{3n})$, the projection of the momentum $p(q(t),\dot q(t))$ onto h is conserved,*

$$p_h(t) := p(q(t),\dot q(t),t)h = \text{const}, \quad t \in [t_0,t_1]. \tag{4.16}$$

Proof 1 The conservation follows from the Noether Theorem for the one-parametric symmetry group $g_s = T_s$ since ph coincides with corresponding Noether invariant. Indeed, the invariant reads

$$I := L_v \frac{d}{ds}\Big|_{s=0} T_s(q) = \sum_i L_{\mathbf{v}_i} \frac{d}{ds}\Big|_{s=0} (\mathbf{q}_i + hs) = \sum_i \mathbf{p}_i h = ph. \tag{4.17}$$ ■

Proof 2 By the definition 4.7, Euler-Lagrange Eqns (3.13), and chain rule of the differentiation,

$$\begin{aligned} \dot p_h(t) = \sum_i \dot{\mathbf{p}}_i(t)h &= -\sum_i \nabla_{\mathbf{q}_i} L(q(t),\dot q(t),t)h \\ &= -\frac{d}{ds}\Big|_{s=0} L(T_s(q(t)), dT_s(q(t),t)\dot q(t)) = 0, \quad t \in [t_0,t_1] \end{aligned} \tag{4.18}$$

by (4.12) and (4.11). ■

4.2.2 Rotation group

Let us fix a unit vector $r \in \mathbb{R}^3$ and consider the transformation R_s from (2.23). By Definition 4.1 the Lagrangian system is invariant with respect to the rotations (2.23) if

$$L(R_s(q), dR_s(q)v, t) = L(q,v,t), \quad (q,v,t) \in \mathcal{E}^+, \quad \forall s \in \mathbb{R}. \tag{4.19}$$

Exercise 4.9 *Check that for the rotations R_s, $s \in \mathbb{R}$, the differential is given by*

$$dR_s(q)v = R_s v, \quad v \in \mathbb{R}^{3n}. \tag{4.20}$$

Exercise 4.10 *Check that the Lagrangian system (2.8) is invariant with respect to the rotations (2.23) with every $r \in \mathbb{R}^3$, if the Lagrangian has the structure (cf. (2.25))*

$$\begin{aligned} L(\mathbf{q}_1,...,\mathbf{q}_n,\mathbf{v}_1,...,\mathbf{v}_n,t) &= \Lambda_1(\{|\mathbf{q}_i - \mathbf{q}_j| : 1 \le i < j \le n;\ |\mathbf{v}_i| : 1 \le i \le n\}, t), \\ &\quad (\mathbf{q}_1,...,\mathbf{q}_n,\mathbf{v}_1,...,\mathbf{v}_n,t) \in \mathcal{E}^+. \end{aligned} \tag{4.21}$$

Definition 4.11 *i) The angular momentum M_i of the i-th particle is the vector-function on the space $\mathcal{E}^+$,*

$$M_i(q,v,t) := \mathbf{q}_i \times \mathbf{p}_i, \quad (q,v,t) \in \mathcal{E}^+. \tag{4.22}$$

ii) the angular momentum M of the Newton system (2.8) is the vector-function on the space $\mathcal{E}^+$,

$$M(q,v,t) := \sum_i M_i = \sum_i \mathbf{q}_i \times \mathbf{p}_i, \quad (q,v,t) \in \mathcal{E}^+. \tag{4.23}$$

Theorem 4.12 *Let the Lagrangian system be invariant with respect to the rotations (2.23) round a fixed vector $r \in \mathbb{R}^3$. Then for any trajectory $q(t) \in C^2([t_0,t_1],\mathbb{R}^{3n})$, the projection of the angular momentum $M(q(t),\dot q(t))$ onto r is conserved,*

$$M_r(t) := M(q(t),\dot q(t))r = \text{const}, \quad t \in [t_0,t_1]. \tag{4.24}$$

Proof 1 The conservation follows from the Noether Theorem for the one-parametric symmetry group $g_s = R_s$ since Mr coincides with corresponding Noether invariant. Indeed, the invariant reads

$$\begin{aligned} I: &= L_v \frac{d}{ds}\Big|_{s=0} R_s(q) = \sum_i L_{v_i} \frac{d}{ds}\Big|_{s=0} (O_r(s)\mathbf{q}_i) \\ &= \sum_i \mathbf{p}_i(r \times \mathbf{q}_i) = \sum_i r(\mathbf{q}_i \times \mathbf{p}_i) = rM \end{aligned} \tag{4.25}$$

according to (2.31). ■

Proof 2 By the definition 4.11, Euler-Lagrange Eqns (3.13) and chain rule of the differentiation,

$$\begin{aligned} \dot{M}_r(t) &= [\sum_i \dot{\mathbf{q}}_i(t) \times \mathbf{p}_i(t) + \sum_i \mathbf{q}_i(t) \times \dot{\mathbf{p}}_i(t)]r \\ &= [\sum_i \dot{\mathbf{q}}_i(t) \times L_{\mathbf{v}_i}(q(t), \dot{q}(t)) + \sum_i \mathbf{q}_i(t) \times L_{\mathbf{q}_i}(q(t), \dot{q}(t))]r \\ &= \sum_i (r \times \dot{\mathbf{q}}_i(t)) L_{\mathbf{v}_i}(q(t), \dot{q}(t)) + \sum_i (r \times \mathbf{q}_i(t)) L_{\mathbf{q}_i}(q(t), \dot{q}(t)). \end{aligned} \tag{4.26}$$

However, (2.31) and (4.20) imply that

$$r \times \mathbf{q}_i(t) = \frac{d}{ds}\Big|_{s=0} O_r(s)\mathbf{q}_i(t), \qquad r \times \dot{\mathbf{q}}_i(t) = \frac{d}{ds}\Big|_{s=0} dO_r(s)\dot{\mathbf{q}}_i(t). \tag{4.27}$$

Therefore, (4.26) implies by the chain rule and (4.19),

$$\dot{M}_r(t) = \frac{d}{dt} L(R_s(q(t)), dR_s(q(t))\dot{q}(t)) = 0. \tag{4.28}$$

■

5 Hamilton Mechanics

5.1 Legendre transform

Let us consider a Lagrangian system with the extended phase space $\mathcal{E}^+ := \mathbb{R}^N \times \mathbb{R}^N \times \mathbb{R}$ and the Lagrangian functional $L \in C^2(\mathcal{E}^+)$. We will identify $\mathbb{R}^N$ with its dual space.

Definition 5.1 *i) The Legendre transform corresponding to the Lagrangian L is the map of the extended phase space $\mathcal{E}^+$ into itself which is defined by $\lambda : (q, v, t) \mapsto (q, p, t)$ with $p := L_v(q, v, t)$. ii) The Legendre transform of the function $L(q, v, t)$ on $\mathcal{E}^+$ is the function on $\lambda\mathcal{E}^+$ defined by $(\Lambda L)(q, p, t) \equiv pv - L(q, v, t)$ with $(q, v, t) = \lambda^{-1}(q, p, t)$, if the Legendre map λ is a C^1-diffeomorphism $\mathcal{E}^+ \to \lambda\mathcal{E}^+$.*

Exercise 5.2 * *Prove that $\lambda : \mathcal{E}^+ \to \lambda\mathcal{E}^+$ is a C^1-diffeomorphism iff the following inequality holds: $|L_{vv}(q, v, t)| \neq 0$, $(q, v, t) \in \mathcal{E}^+$.*

Example 5.3 *The inequality holds for the Lagrangian (3.14) because then the Jacobian matrix $J := L_{vv}(q, v, t)$ is diagonal and $|J| = m_1 ... m_n \neq 0$ since all $m_i > 0$.*

Example 5.4 $\Lambda v^2 = p^2/4$, $\Lambda v^4 = 3v^4 = 3(p/4)^{4/3}$,...

Exercise 5.5 *Prove that $\Lambda(\Lambda L) = L$ if $\lambda : \mathcal{E}^+ \to \lambda\mathcal{E}^+$ is a C^1-diffeomorphism.*

Theorem 5.6 *Let the Legendre transform Λ be a C^1-diffeomorphism $\mathcal{E}^+ \to \Lambda\mathcal{E}^+$. Then Λ transforms the Euler-Lagrange Eqns (3.15) into the Hamiltonian form,*

$$\dot{q}(t) = H_p(q(t), p(t), t), \qquad \dot{p}(t) = -H_q(q(t), p(t), t), \tag{5.1}$$

where $H(q, p, t)$ is the Legendre transform of the Lagrangian,

$$H(q, p, t) = pv - L(q, v, t), \qquad p = L_v(q, v, t). \tag{5.2}$$

Proof The first equation of (5.1) follows by differentiation of the identity $H(q, p, t) \equiv pv - L(q, v, t)$:

$$H_p = v + pv_p - L_q q_p - L_v v_p = v = \dot{q} \tag{5.3}$$

since $p = L_v$ by definition, and $q_p = 0$. The second equation of (5.1) follows from the Euler-Lagrange Eqn (3.15):

$$H_q = p_q v + pv_q - L_q - L_v v_q = -L_q = -\dot{p}. \tag{5.4}$$

since $p = L_v$ by definition, and $p_q = 0$. ■

Remark 5.7 *In (5.3) and (5.4) the derivatives L_q mean the derivative with fixed v and t but in all other terms the derivatives in q mean the derivatives with fixed p and t.*

Example 5.8 *For the Lagrangian (3.14) the energy has the form (3.18), hence $H(q, p, t) = \sum_i \frac{\mathbf{p}_i^2}{2m_i} + V(q, t)$.*

Exercise 5.9 *Calculate the momentum, energy and the Hamilton function for the Lagrangian*

$$L(\mathbf{q}, \mathbf{v}) = -m\sqrt{1 - \mathbf{v}^2}, \quad (\mathbf{q}, \mathbf{v}) \in \mathbb{R}^3 \times \mathbb{R}^3. \tag{5.5}$$

Solution:

$$p := m\mathbf{v}/\sqrt{1 - \mathbf{v}^2}, \qquad \mathbf{v} = \mathbf{p}/\sqrt{m^2 + \mathbf{p}^2}, \qquad E = m/\sqrt{1 - \mathbf{v}^2}, \qquad H = \sqrt{m^2 + \mathbf{p}^2}. \tag{5.6}$$

5.2 Hamilton-Jacobi Equation

Let us consider the Lagrangian function $L(q,v,t) \in C^2(\mathcal{E}^+)$ with the corresponding Hamilton function $H(q,p,t) \in C^2(\mathcal{E}^+)$ on the extended phase space $\mathcal{E}^+ := \mathbb{R}^N \times \mathbb{R}^N \times \mathbb{R}$ and the Cauchy problem of the type

$$\left.\begin{aligned} -\dot S(t,x) &= H(x, \nabla S(t,x), t), \quad (t,x) \in \mathbb{R}^{N+1} \\ S|_{t=0} &= S_0(x), \quad x \in \mathbb{R}^N, \end{aligned}\right| \tag{5.7}$$

where $S_0(x) \in C^1(\mathbb{R}^N)$ is a given function. Let us describe the Hamilton-Jacobi method of the construction of the solution to the problem (5.7).

First, consider the corresponding Cauchy problem for the Hamilton system,

$$\left.\begin{aligned} \dot q(t) &= H_p(q(t),p(t),t), & \dot p(t) &= -H_q(q(t),p(t),t) \\ q|_{t=0} &= q_0, & p|_{t=0} &= \nabla S_0(q_0) \end{aligned}\right| \tag{5.8}$$

with $q_0 \in \mathbb{R}^N$. Let us denote the solution by $(q(t,q_0), p(t,q_0))$. The solution exists and is C^1-smooth for small $|t|$ depending on q_0. Let us define the function $\mathcal{S}$ by the action integral

$$\mathcal{S}(t,q_0) = S_0(q_0) + \int_0^t L(q(s,q_0), \dot q(s,q_0), s)ds \tag{5.9}$$

for $q_0 \in \mathbb{R}^N$ and small $|t|$. At last, let us express q_0 in $q(t,q_0)$ for small $|t|$: this is possible since the Jacobian $q_{q_0}(t,q_0) = E$ for $t = 0$. Thus, $q_0 = q_0(t,q)$ where $q_0(t,q) \in C^1(\mathbb{R} \times \mathbb{R}^N)$, hence we can define

$$S(t,x) = \mathcal{S}(t, q_0(t,x)), \quad x \in \mathbb{R}^N \tag{5.10}$$

for small $|t|$.

Theorem 5.10 *Let $T > 0$ and the map $q_0 \mapsto q(t,q_0)$ be C^1-diffeomorphism of $\mathbb{R}^N$ for $t \in [0,T]$. Then the function $S(t,x)$ from (5.10) is the unique solution to the Cauchy problem (5.7) for $t \in [0,T]$.*

Proof The theorem follows from the properties of the differential 1-form $\omega^1 = pdq - Hdt$ in $\mathbb{R}^{N+1}$ called as the *Poincaré-Cartan integral invariant* [1].

Step i) Let us consider $q_0, q_0 + \Delta q_0 \in \mathbb{R}^N$ and $\tau, \tau + \Delta\tau \in [0,T]$. Let $\mathcal{M}_\tau$ denote two-dimensional submanifold in the extended phase space $\mathcal{E}^+$.

$$\mathcal{M}_\tau = \{q(t, q_0 + s\Delta q_0), q(t, q_0 + s\Delta q_0), t) : s \in [0,1], t \in [0, \tau + s\Delta\tau]\}. \tag{5.11}$$

The boundary $\partial\mathcal{M}_\tau$ is the union $\alpha \cup \gamma_1 \cup \beta \cup \gamma_2$, where

$$\left.\begin{aligned} \alpha &:= \{(q_0 + s\Delta q_0, \nabla S_0(q_0 + s\Delta q_0), 0) : s \in [0,1]\}, \\ \beta &:= \{(q(t + s\Delta\tau, (q_0 + s\Delta q_0)), p(t + s\Delta\tau, (q_0 + s\Delta q_0)), t + s\Delta\tau) : s \in [0,1]\}, \\ \gamma_0 &:= \{(q(t,q_0)), p(t,q_0), t) : t \in [0,\tau]\}, \\ \gamma_1 &:= \{(q(t, q_0 + \Delta q_0)), p(t, q_0 + \Delta q_0), t) : t \in [0, \tau + \Delta\tau]\} \end{aligned}\right| \tag{5.12}$$

are oriented according to the increment of the parameters s,t. Therefore by the Stokes Theorem,

$$\int\limits_{\mathcal{M}_\tau} d\omega^1 = \int\limits_{\alpha} \omega^1 + \int\limits_{\gamma_1} \omega^1 - \int\limits_{\beta} \omega^1 - \int\limits_{\gamma_0} \omega^1. \tag{5.13}$$

Step ii) Central point of the proof is the observation that the restriction of the form $d\omega^1$ onto the submanifold $\mathcal{M}_\tau$ vanishes,

$$d\omega^1|_{\mathcal{M}_\tau} = 0. \tag{5.14}$$

This follows from two facts: i) the Hamilton vector field $\mathcal{H} := (H_p, -H_q, 1)$ in the extended phase space $\mathcal{E}^+$ is tangent to $\mathcal{M}_\tau$ at every point, and ii) $d\omega^1(\mathcal{H}, \mathcal{V}) \equiv 0$ for every vector field $\mathcal{V}$ in $\mathcal{E}^+$. The last identity follows by the following calculations: first, $d\omega^1 = dp \wedge dq - dH \wedge dt = dp \wedge dq - (H_p dp + H_q dq) \wedge dt$ is the antisymmetric bilinear form with the matrix

$$A = \begin{pmatrix} 0 & E & H_q \\ -E & 0 & H_p \\ -H_q & -H_p & 0 \end{pmatrix}, \tag{5.15}$$

where E is the identity $N \times N$-matrix. Second, $A\mathcal{H} \equiv 0$, hence

$$d\omega^1(\mathcal{H}, \mathcal{V}) = \langle A\mathcal{H}, \mathcal{V} \rangle \equiv 0. \tag{5.16}$$

Step iii) Now (5.13) reads,

$$\int_\beta (p dq - H dt) = \int_\alpha \nabla S_0(q) dq + \int_{\gamma_1} L dt - \int_{\gamma_0} L dt \tag{5.17}$$

since $dt|_\alpha = 0$, $p|_\alpha = \nabla S_0(q)$ and $\omega^1|_{\gamma_i} = L dt$. The first term in the RHS of (5.17) equals to $S_0(q_0 + \Delta q_0) - S_0(q_0)$. Therefore, (5.17) becomes by the definitions (5.9), (5.10),

$$\begin{aligned} \int_\beta (p dq - H dt) &= S_0(q_0 + \Delta q_0) + \int_{\gamma_1} L dt - (S_0(q_0) + \int_{\gamma_0} L dt) \\ &= S(q + \Delta q, \tau + \Delta\tau) - S(q, \tau) \end{aligned} \tag{5.18}$$

where $q + \Delta q = q(\tau + \Delta\tau, q_0 + \Delta q_0)$ and $q = q(\tau, q_0)$. Finally, (5.18) implies $\dot{S}(t, q) = -H(q, p, t)$ and $\nabla S(t, q) = p$, hence the equation (5.9) follows. ■

6 Euler-Lagrange Field Equations

6.1 Nonlinear Klein-Gordon and Schrödinger Equations

Let us define $x_0 = ct$, $\mathbf{x} = (x_1, x_2, x_3)$, $x = (x_0, \mathbf{x})$ and consider the *nonlinear* Klein-Gordon and Schrödinger Equation

$$\begin{aligned} &(i\hbar\nabla_0 - \not{e}\phi(x))^2\psi(x) \\ &= (-i\hbar\nabla_{\mathbf{x}} - \not{e}A(x))^2\psi(x) + m^2c^2\psi(x) - F(\psi(x)), \qquad x \in \mathbb{R}^4, \end{aligned} \tag{6.1}$$

where the function $\psi(x)$ takes complex values and $F \in C^1(\mathbb{C}, \mathbb{C})$. Let us consider also the nonlinear Schrödinger Equation

$$\begin{aligned} &(i\hbar\nabla_0 - e\phi(x))\psi(x) \\ &= \frac{1}{2m}(-i\hbar\nabla_{\mathbf{x}} - \not{e}A(x)))^2\psi(x) - F(\psi(x)), \qquad x \in \mathbb{R}^4, \end{aligned} \tag{6.2}$$

where $x_0 := t$.

6.2 Lagrangian density

Definition 6.1 *We will identify the complex vectors $\psi \in \mathbb{C}^M$ with the real vectors $\mathbb{R}\psi := (\Re\psi, \Im\psi) \in \mathbb{R}^{2M}$ and the multiplication by a complex number with an application of the corresponding matrix. We will denote by $\cdot$ the real scalar product in $\mathbb{R}^{2M}$.*

This definition implies the formulas

$$\mathbb{R}u \cdot \mathbb{R}v = \Re(u\overline{v}), \tag{6.3}$$

$$\nabla_{\mathbb{R}u}(u \cdot iv) = iv, \quad \nabla_{\mathbb{R}v}(u \cdot iv) = -iu, \qquad \nabla_{\mathbb{R}u}(iu \cdot v) = -iv, \quad \nabla_{\mathbb{R}v}(iu \cdot v) = iu, \tag{6.4}$$

for $u, v \in \mathbb{C}$ since $u \cdot iv = -iu \cdot v$ and $iu \cdot v = -u \cdot iv$. We will assume that

$$F(\psi) = -\nabla_\psi U(\psi), \quad \psi \in \mathbb{C}, \tag{6.5}$$

where $U \in C^2(\mathbb{C})$ and ∇_ψ stands for the gradient with respect to the real and imaginary part of ψ.

Let us introduce the *Lagrangian density* $\mathcal{L}$ for the Eqn (6.1) resp. (6.2) as the function defined resp. by (cf. (2.3), (2.10)),

$$\begin{aligned} \mathcal{L}_{KG}(x, \psi, \nabla\psi) &= \frac{|(i\hbar\nabla_0 - \not{e}\phi(x))\psi|^2}{2} - \sum_{k=1}^{3}\frac{|(-i\hbar\nabla_k - \not{e}A_k(x))\psi|^2}{2} \\ &\quad -m^2c^2\frac{|\psi|^2}{2} - U(\psi), \end{aligned} \tag{6.6}$$

$$\begin{aligned} \mathcal{L}_S(x, \psi, \nabla\psi) &= \frac{(i\hbar\nabla_0 - e\phi(x))\psi \cdot \psi}{2} - \frac{1}{2m}\sum_{k=1}^{3}\frac{|(-i\hbar\nabla_k - \not{e}A_k(x))\psi|^2}{2} \\ &\quad -U(\psi). \end{aligned} \tag{6.7}$$

We will demonstrate below that the field equations (6.1), (6.2) can be represented in the **Euler-Lagrange** form,

$$\mathcal{L}_\psi(x,\psi(x),\nabla\psi(x)) - \sum_{\alpha=0}^{3}\nabla_\alpha\mathcal{L}_{\nabla_\alpha\psi}(x,\psi(x),\nabla\psi(x)) = 0, \quad x\in\mathbb{R}^4, \tag{6.8}$$

where $\mathcal{L}$ is the corresponding Lagrangian density.

Remark 6.2 *In (6.6) – (6.8) the x and $\psi, \nabla_\alpha\psi$ are considered as independent variables with the values in $\mathbb{R}^4$ and $\mathbb{R}^2$ respectively.*

Definition 6.3 *The Lagrangian field $\psi(x)$ with values in $\mathbb{R}^N$ is the dynamical system described by the N real scalar equations (6.8) with a given Lagrangian density $\mathcal{L}(x,\psi,\nabla\psi) \in C^2(\mathbb{R}^4\times\mathbb{R}^N\times\mathbb{R}^{4N})$.*

Definition 6.4 *The* **canonically conjugate fields** *$\pi_\alpha(x)$ are defined by*

$$\pi_\alpha(x) = \mathcal{L}_{\nabla_\alpha\psi}(x,\psi(x),\nabla\psi(x)), \quad \alpha = 0,...,3. \tag{6.9}$$

With these notations the Euler-Lagrange Equations (6.8) read

$$\nabla_\alpha\pi_\alpha(x) = \mathcal{L}_\psi(x,\psi(x),\nabla\psi(x)), \quad x\in\mathbb{R}^4. \tag{6.10}$$

Here and below we suggest the Einstein convention $\nabla_\alpha\pi_\alpha(x) := \sum_\alpha \nabla_\alpha\pi_\alpha(x)$ etc. Also $\alpha = 0,1,2,3$ and $k = 1,2,3$.

6.3 Free linear equations

First consider *free* linear equations without Maxwell Field and nonlinear selfaction, and with $\hbar = 1$:

$$\begin{aligned}\nabla_0^2\psi(x) &= \nabla_{\mathbf{x}}^2\psi(x) - m^2c^2\psi(x), \qquad x\in\mathbb{R}^4,\\ -i\nabla_0\psi(x) &= \frac{1}{2m}\nabla_{\mathbf{x}}^2\psi(x), \qquad x\in\mathbb{R}^4,\end{aligned} \tag{6.11}$$

Then the Lagrangian densities (6.6), (6.7) become

$$\mathcal{L}^0_{KG}(x,\psi,\nabla\psi) = \frac{|\nabla_0\psi|^2}{2} - \sum_{k=1}^{3}\frac{|\nabla_k\psi|^2}{2} - m^2c^2\frac{|\psi|^2}{2}, \tag{6.12}$$

$$\mathcal{L}^0_{S}(x,\psi,\nabla\psi) = \frac{i\nabla_0\psi\cdot\psi}{2} - \frac{1}{2m}\sum_{k=1}^{3}\frac{|\nabla_k\psi|^2}{2} \tag{6.13}$$

Exercise 6.5 *Check the Euler-Lagrange form (6.10) for the Klein-Gordon and Schrödinger Equations (6.11), (6.11).*

Solution
I For the Klein-Gordon Eqn (6.11): by the formulas (6.4) we get

$$\pi_0(x) = \nabla_0\psi(x), \quad \pi_k(x) = -\nabla_k\psi(x), \qquad \mathcal{L}_\psi = -m^2\psi. \tag{6.14}$$

Hence (6.10) is equivalent to (6.11).
II For the Schrödinger Eqn (6.11): by the formulas (6.4) we get

$$\pi_0(x) = -\frac{i\psi(x)}{2}, \quad \pi_k(x) = -\frac{1}{2m}\nabla_k\psi(x), \quad \mathcal{L}_\psi = -\frac{i\nabla_0\psi(x)}{2}. \tag{6.15}$$

Hence (6.10) is equivalent to (6.11).

6.4 Nonlinear equations with Maxwell Field

Exercise 6.6 *Check the Euler-Lagrange form (6.10) for the Klein-Gordon and Schrödinger Equations (6.1), (6.2).*

Solution
I For the Klein-Gordon Eqn (6.1): by the formulas (6.4) we get

$$\text{(6.16)}\quad \begin{cases} \pi_0(x) = -i\hbar(i\hbar\nabla_0 - \not\phi(x))\psi(x), \quad \pi_k(x) = -i\hbar(-i\hbar\nabla_k - \not A_k(x))\psi(x), \\ \mathcal{L}_\psi \quad = -\not\phi(x)(i\hbar\nabla_0 - \not\phi(x))\psi(x) + \not A_k(x)(-i\hbar\nabla_k - \not A_k(x))\psi(x) - m^2\psi + F(\psi). \end{cases}$$

Hence (6.10) is equivalent to (6.1).
II For the Schrödinger Eqn (6.2): by the formulas (6.4) we get

$$\text{(6.17)}\quad \begin{cases} \pi_0(x) \quad = -\dfrac{i\hbar\psi(x)}{2}, \quad \pi_k(x) = -\dfrac{1}{2m} i\hbar(-i\hbar\nabla_k - \not A_k(x))\psi(x), \\ \mathcal{L}_\psi \quad = e\phi(x)\psi(x) - \dfrac{i\hbar\nabla_0\psi(x)}{2} + \dfrac{1}{2m}\not A_k(x)(-i\hbar\nabla_k - \not A_k(x))\psi(x) + F(\psi). \end{cases}$$

Hence (6.10) is equivalent to (6.2).

6.5 Action functional

Definition 6.7 *For $k = 1, 2, ...$ and $\sigma > 0$ the space C^k_σ is the set of the functions $\psi(t, \mathbf{x}) \in C^k([0, \infty) \times \mathbb{R}^3, \mathbb{R}^N)$ with the space-decay*

$$\text{(6.18)}\qquad \sum_{|\alpha| \le k} |\nabla^\alpha \psi(t, \mathbf{x})| \le C_T(1 + |\mathbf{x}|)^{-\sigma}, \quad (t, \mathbf{x}) \in C^k([0, T] \times \mathbb{R}^3).$$

We will consider the real-valued functionals $\mathcal{F}$ on C^1_σ. By definition, $\mathcal{F}$ is a map $C^1_\sigma \to \mathbb{R}$.

Definition 6.8 *For $\psi \in C^1_\sigma$ the Gateau derivative $D\mathcal{F}(\psi)$ is the* **linear** *functional defined by*

$$\text{(6.19)}\qquad \langle D\mathcal{F}(\psi), h\rangle = \frac{d}{d\varepsilon}\Big|_{\varepsilon=0} \mathcal{F}(\psi + \varepsilon h)$$

for $h(\cdot) \in C^1_\sigma$ if the derivative exists.

We will assume the following bounds for the Lagrangian density,

$$\text{(6.20)}\qquad \left.\begin{array}{rcl} |\mathcal{L}(x, \psi, \nabla\psi)| & \le & C(|\psi| + |\nabla\psi|)^2 \\ |\mathcal{L}_\psi(x, \psi, \nabla\psi)| + |\mathcal{L}_{\nabla\psi}(x, \psi, \nabla\psi)| & \le & C(|\psi| + |\nabla\psi|) \end{array}\right|, \quad |\psi| + |\nabla\psi| \le \text{const}.$$

Let us fix a $T > 0$.

Definition 6.9 *The action for the field is the function for the field is the functional on C^1_σ, $\sigma > 3/2$ defined by*

$$\text{(6.21)}\qquad S_T(\psi) = \int_0^T [\int_{\mathbb{R}^3} \mathcal{L}(x, \psi(x), \nabla\psi(x))d\mathbf{x}]dx_0, \quad \psi(\cdot) \in C^1_\sigma.$$

Note that for $\sigma > 3/2$ the action is defined on the whole of C^1_σ by (6.18) and the first inequality of (6.20). Moreover, the functional is differentiable:

Lemma 6.10 *The Gateau derivative* $\langle DS_T(\psi), h\rangle$ *exists for* $\psi, h \in C^1_\sigma$ *if* $\sigma > 3/2$.

Proof From definition 6.8 we get by the theorem of the differentiation of the integrals,

$$\langle DS_T(\psi), h\rangle := \frac{d}{d\varepsilon}\Big|_{\varepsilon=0} \int_0^T [\int_{\mathbb{R}^3} \mathcal{L}(x, \psi(x) + \varepsilon h(x), \nabla\psi(x) + \varepsilon\nabla h(x))d\mathbf{x}]dx_0$$

$$= \int_0^T [\int_{\mathbb{R}^3} \Big(\mathcal{L}_\psi(x, \psi(x), \nabla\psi(x))h(x) + \sum_{\alpha=0}^{3} \mathcal{L}_{\nabla_\alpha\psi}(x, \psi(x), \nabla\psi(x))\nabla_\alpha h(x)\Big)d\mathbf{x}]dx_0 \tag{6.22}$$

since the integrals converge uniformly by (6.18) and (6.20). ■

6.6 The Hamilton Least Action Principle

Let us introduce the space of *variations*.

Definition 6.11 $C^1(T)$ *is the space of functions* $h(\cdot) \in C^1([0,T] \times \mathbb{R}^3, \mathbb{R}^N)$ *such that*

$$h(0, \mathbf{x}) = h(T, \mathbf{x}) = 0, \ \mathbf{x} \in \mathbb{R}^3, \tag{6.23}$$

$$h(t, \mathbf{x}) = 0, \quad |\mathbf{x}| \geq \text{const}, \ t \in [0, T]. \tag{6.24}$$

Definition 6.12 *The function* $\psi \in C^1_\sigma$ *satisfies the Hamilton Least Action Principle (LAP) if for any* $T > 0$,

$$\langle DS_T(\psi), h\rangle = 0, \quad \forall h(\cdot) \in C^1(T). \tag{6.25}$$

Theorem 6.13 *For* $\psi \in C^2_\sigma$ *with* $\sigma > 3/2$ *the Hamilton LAP is equivalent to the Euler-Lagrange Eqns (6.8).*

Proof (6.22) implies by partial integration in x_α, $\alpha = 0, ..., 3$,

$$\langle DS_T(\psi), h\rangle$$

$$\int_0^T [\int_{\mathbb{R}^3} \Big(\mathcal{L}_\psi(x, \psi(x), \nabla\psi(x))h(x) - \sum_{\alpha=0}^{3} \nabla_\alpha\mathcal{L}_{\nabla_\alpha\psi}(x, \psi(x), \nabla\psi(x))\Big)h(x)d\mathbf{x}]dx_0. \tag{6.26}$$

Therefore, (6.25) is equivalent to (6.8) by the Main Lemma of the Calculus of Variations. ■

Remark 6.14 *The expositions in Sections 3.1, 3.2 and 6.3 formally are similar.*

7 Energy and momentum currents

Let us show that the invariance of the Lagrangian density with respect to translations in time and space leads to the energy and momentum conservation.

7.1 Energy and momentum

Let us fix a $\sigma > 3/2$.

Definition 7.1 *(cf. Definitions 3.3, 3.18) i) The energy of the Lagrangian field $\psi(x) \in C^1_\sigma$ is defined by*

$$E(t) = \int_{\mathbb{R}^3} \Big[\pi_0(x)\nabla_0\psi(x) - \mathcal{L}(x,\psi(x),\nabla\psi(x))\Big]\Big|_{x_0=ct} d\mathbf{x}, \quad t \in \mathbb{R}. \tag{7.1}$$

ii) The momentum of the Lagrangian field at time t is the vector with the components

$$P_k(t) = -\int_{\mathbb{R}^3} \Big[\pi_0(x)\,\nabla_k\psi(x)\Big]\Big|_{x_0=ct} d\mathbf{x}, \quad k = 1,2,3, \quad t \in \mathbb{R}. \tag{7.2}$$

Remark 7.2 *By definition, $\pi_0(x)\,\nabla_k\psi(x) = \pi_0^j(x)\,\nabla_k\psi^j(x)$.*

Note that by (6.18) and (6.20) the energy and momentum are well defined for the solutions $\psi(t) \in C^1_\sigma$ since $\sigma > 3/2$.

Example 7.3 *The linear one-dimensional d'Alembert Eqn*

$$\ddot\psi(t,\mathbf{x}) = \psi''(t,\mathbf{x}), \quad \mathbf{x} \in \mathbb{R} \tag{7.3}$$

is a particular case of the nonlinear Klein-Gordon Eqn (6.1). Then the Lagrangian density $\mathcal{L}$ is given by (6.6), i.e.

$$\mathcal{L}(t,\mathbf{x},\psi,\dot\psi,\psi') = \frac{|\dot\psi|^2}{2} - \frac{|\psi'|^2}{2}. \tag{7.4}$$

Then the canonically conjugates are $\pi_0 = \dot\psi$ and $\pi_k = -\nabla_k\psi$. Hence the energy and momentum are given by

$$E(t) = \int_{\mathbb{R}} \Big[\frac{|\dot\psi(t,\mathbf{x})|^2}{2} + \frac{|\psi'(t,\mathbf{x})|^2}{2}\Big] d\mathbf{x}, \quad t \in \mathbb{R}. \tag{7.5}$$

$$P(t) = -\int_{\mathbb{R}} \dot\psi(t,\mathbf{x})\,\psi'(t,\mathbf{x})\,d\mathbf{x}, \qquad t \in \mathbb{R}. \tag{7.6}$$

7.2 Invariance in time and energy conservation

Theorem 7.4 *Let the Lagrangian density $\mathcal{L}$ do not depend on $x_0 := ct$,*

$$\mathcal{L}(x,\psi,\nabla\psi) \equiv \mathcal{L}_1(\mathbf{x},\psi,\nabla\psi). \tag{7.7}$$

Then for any trajectory $\psi(x) \in C^2_\sigma$ of the equations (6.10) the energy is conserved, $E(t) =$const.

Proof for a particular case Let us prove the theorem for the d'Alembert Eqn (7.3).

By definition (7.5), $E(t) = \lim_{R\to\infty} E_R(t)$ where

$$E_R(t) = \int_{-R}^{R} \Big[\frac{|\dot\psi(t,\mathbf{x})|^2}{2} + \frac{|\psi'(t,\mathbf{x})|^2}{2}\Big] d\mathbf{x}. \tag{7.8}$$

Differentiating, we get

$$\dot E_R(t) = \int_{-R}^{R} \Big[\dot\psi(t,\mathbf{x})\ddot\psi(t,\mathbf{x}) + \psi'(t,\mathbf{x})\dot\psi'(t,\mathbf{x})\Big] d\mathbf{x}. \tag{7.9}$$

Substituting $\ddot\psi(t,\mathbf{x}) = \psi''(t,\mathbf{x})$ from (7.3), we get by partial integration,

$$\dot E_R(t) = \Big[\dot\psi(t,\mathbf{x})\psi'(t,\mathbf{x})\Big]\Big|_{-R}^{R} = \mathcal{P}(t,-R) - \mathcal{P}(t,R), \tag{7.10}$$

where $\mathcal{P}(t,\mathbf{x}) := -\dot\psi(t,\mathbf{x})\psi'(t,\mathbf{x})$. Now (6.18) implies that for every fixed t we have $\dot E_R(t) \to 0$ as $R\to\infty$, hence $E(t)$ =const. Indeed, for any $T > 0$,

$$E_R(T) - E_R(0) = \int_0^T \dot E_R(t)dt, \tag{7.11}$$

hence in the limit $R\to\infty$,

$$E(T) - E(0) = \int_0^T \lim_{R\to\infty} \dot E_R(t)dt = 0. \tag{7.12}$$ ■

Remark 7.5 *The identity (7.10) means that the* **momentum density** $\mathcal{P}(t,\mathbf{x})$ *coincides with the* **energy current density**.

Proof for the general case By definition (7.1), $E(t) = \lim_{R\to\infty} E_R(t)$ where

$$E_R(t) = \int_{|\mathbf{x}|<R} \Big[\pi_0(x)\nabla_0\psi(x) - \mathcal{L}(x,\psi(x),\nabla\psi(x))\Big]\Big|_{x_0=ct} d\mathbf{x}. \tag{7.13}$$

Differentiating, we get

$$\begin{aligned}\dot E_R(t) = \int_{|\mathbf{x}|<R} \Big[&\nabla_0\pi_0(x)\nabla_0\psi(x) + \pi_0(x)\nabla_0^2\psi(x)\\ &-\mathcal{L}_\psi(x,\psi(x),\nabla\psi(x))\nabla_0\psi(x) - \sum_{\alpha=0}^{3}\pi_\alpha(x)\nabla_0\nabla_\alpha\psi\Big]\Big|_{x_0=ct} d\mathbf{x}.\end{aligned} \tag{7.14}$$

By (6.10) we have $\nabla_0\pi_0(x) = \mathcal{L}_\psi(x,\psi(x),\nabla\psi(x)) - \sum_1^3 \nabla_k\pi_k(x)$. Substituting into (7.14), we get by the Stokes Theorem,

$$\begin{aligned}\dot E_R(t) &= -\int_{|\mathbf{x}|<R} \Big[\sum_1^3 \nabla_k\pi_k(x)\nabla_0\psi + \sum_{\alpha=1}^{3}\pi_\alpha(x)\nabla_0\nabla_\alpha\psi\Big]\Big|_{x_0=ct} d\mathbf{x}\\ &= -\int_{|\mathbf{x}|<R} \sum_1^3 \nabla_k\Big[\pi_k(x)\nabla_0\psi(x)\Big]\Big|_{x_0=ct} d\mathbf{x}\\ &= -\int_{|\mathbf{x}|=R} \sum_1^3 n_k(\mathbf{x})\Big[\pi_k(x)\nabla_0\psi(x)\Big]\Big|_{x_0=ct} dS,\end{aligned} \tag{7.15}$$

where $n_k(\mathbf{x}) := x_k/|\mathbf{x}|$ and dS is the Lebesgue measure on the sphere $|\mathbf{x}| = R$. Now (6.18) implies that for every fixed t we have $\dot{E}_R(t) \to 0$ as $R \to \infty$, hence $E(t)$ =const. ■

Remark 7.6 *The identity (7.15) means that the vector-function*

$$S_k(x) := \pi_k(x)\nabla_0\psi(x) := \pi_k^j(x)\nabla_0\psi^j(x), \qquad k = 1, ..., 3, \quad x \in \mathbb{R}^4 \tag{7.16}$$

is the **energy current density** *in the field $\psi(x)$.*

7.3 Invariance in space and momentum conservation

Theorem 7.7 *Let the Lagrangian density $\mathcal{L}$ do not depend on x_1,*

$$\mathcal{L}(x, \psi, \nabla\psi) \equiv \mathcal{L}_2((x_0, x_2, x_3), \psi, \nabla\psi). \tag{7.17}$$

*Then for any trajectory $\psi(x) \in C_\sigma^2$ of the equations (6.10) the first component of the momentum is conserved, $P_1(t)$ =*const.

Proof for a particular case Let us prove the theorem for the d'Alembert Eqn (7.3). By definition, $P(t) = \lim_{R\to\infty} P_R(t)$ where

$$P_R(t) = -\int_{-R}^{R} \dot{\psi}(t, \mathbf{x})\psi'(t, \mathbf{x})d\mathbf{x}. \tag{7.18}$$

Differentiating, we get

$$\dot{P}_R(t) = -\int_{-R}^{R} \Big[\ddot{\psi}(t, \mathbf{x})\psi'(t, \mathbf{x}) + \dot{\psi}(t, \mathbf{x})\dot{\psi}'(t, \mathbf{x})\Big] d\mathbf{x}. \tag{7.19}$$

Substituting $\ddot{\psi}(t, \mathbf{x}) = \psi''(t, \mathbf{x})$ from (7.3), we get,

$$\dot{P}_R(t) = -\Big[\frac{|\psi'(t, \mathbf{x})|^2}{2} + \frac{|\dot{\psi}(t, \mathbf{x})|^2}{2}\Big]\Big|_{-R}^{R} = \mathcal{E}(t, -R) - \mathcal{E}(t, R), \tag{7.20}$$

where $\mathcal{E}(t, \mathbf{x}) := \dfrac{|\psi'(t, \mathbf{x})|^2}{2} + \dfrac{|\dot{\psi}(t, \mathbf{x})|^2}{2}$. Now (6.18) implies that for every fixed t we have $\dot{P}_R(t) \to 0$ as $R \to \infty$, hence $P(t)$ =const. ■

Remark 7.8 *The identity (7.20) means that the* **energy density** $\mathcal{E}(t, \mathbf{x})$ *coincides with the* **momentum current density**.

Exercise 7.9 *Prove Theorem 7.7 for the general case.*

Exercise 7.10 *Calculate the current of P_1 in the field.*

8 Angular momentum and charge currents

The energy and momentum conservation holds for the Lagrangian fields with values in $\mathbb{R}^N$ for any $N \geq 1$. These conservations are related to the invariance of the Lagrangian density $\mathcal{L}$ with respect to the translations in time and space. Now consider the Lagrangian densities $\mathcal{L}$ which are invariant with respect to different rotation groups.

8.1 Space rotations and angular momentum conservation

Let us consider the rotations $O_3(s)$ of the space $\mathbb{R}^3$ round a unit vector $e_3 := (0,0,1) \in \mathbb{R}^3$ with the angle of s *radian*. Let us consider the Lagrangian densities which are invariant with respect to the space-rotations round the vector e_3:

$$\begin{aligned} &\mathcal{L}(x,\psi(x),\nabla\psi(x)) \equiv \mathcal{L}_*(x_0,|(x_1,x_2)|,x_3,|\psi(x)|,\\ &|(\nabla_2\psi(x),\nabla_2\psi(x))|,x_1\nabla_1\psi(x)+x_2\nabla_2\psi(x),x_2\nabla_1\psi(x)-x_1\nabla_2\psi(x),\nabla_3\psi(x)). \end{aligned} \tag{8.1}$$

Let us fix a $\sigma > 2$.

Definition 8.1 *(cf. Definitions 2.14, 4.11, 7.2) The angular momentum of the Lagrangian field at time t is the vector with the components*

$$M_k(t) = \int_{\mathbb{R}^d} \Big[\pi_0(x)\ (\mathbf{x}\times\nabla_{\mathbf{x}})_k\psi(x)\Big]\Big|_{x_0=ct} d\mathbf{x}, \quad k=1,2,3, \quad t\in\mathbb{R}, \tag{8.2}$$

where $\nabla_{\mathbf{x}} := (\nabla_1,\nabla_2,\nabla_3)$: for example, $(\mathbf{x}\times\nabla_{\mathbf{x}})_3 := x_1\nabla_2 - x_2\nabla_1$ etc.

Note that the integral converges for the solutions $\psi(t) \in C^1_\sigma$ with $\sigma > 2$ by (6.18) and (6.20).

Remark 8.2 *By definition, $\pi_0(x)\ (\mathbf{x}\times\nabla_{\mathbf{x}})_k\psi(x) = \pi_0^j(x)\ (\mathbf{x}\times\nabla_{\mathbf{x}})_k\psi^j(x)$.*

Theorem 8.3 *Let the Lagrangian density satisfy (8.1) and $\sigma > 5/2$. Then for any trajectory $\psi(x) \in C^2_\sigma$ of the equations (6.10) the third component of the angular momentum is conserved, $M_3(t)$ =const.*

Exercise 8.4 *Prove Theorem 8.3.*

Exercise 8.5 *Calculate the current density of the M_3 in the field.*

Exercise 8.6 *Calculate the angular momentum for the Klein-Gordon and Schrödinger Equations (6.1), (6.2).*

8.2 Internal rotations and charge conservation

Consider complex-valued fields ψ with Lagrangian densities which are invariant with respect to the rotations in ψ:

$$\mathcal{L}(x,\psi(x),\nabla\psi(x)) \equiv \mathcal{L}_*(x,|\psi(x)|,|\nabla_0\psi(x)|,|\nabla_1\psi(x)|,|\nabla_2\psi(x)|,|\nabla_3\psi(x)|). \tag{8.3}$$

Exercise 8.7 *Check that (8.3) holds for Eqns (6.1) and (6.2) if $U(\psi)$ depends only on $|\psi|$.*

Let us fix a $\sigma > 3/2$.

Definition 8.8 *The charge of the Lagrangian field at time t is defined by*

$$Q(t) = \int_{\mathbb{R}^d} \Big[\pi_0(x) \cdot i\psi(x)\Big]\Big|_{x_0=ct} d\mathbf{x}, \qquad t \in \mathbb{R}, \tag{8.4}$$

where $\pi_0(x)$ and $i\psi(x)$ are identified with the real vectors from $\mathbb{R}^2$, and $\cdot$ is the real scalar product in $\mathbb{R}^2$ (cf. (6.4)).

Note that the integral converges for the solutions $\psi(t) \in C^1_\sigma$ by (6.18) and (6.20) since $\sigma > 3/2$.

Theorem 8.9 *Let the Lagrangian density satisfy (8.3) and $\sigma > 3/2$. Then for any trajectory $\psi(x) \in C^2_\sigma$ of the equations (6.10) the charge is conserved, $Q(t)$ =const.*

Proof for a particular case Let us prove the theorem for the *free linear* 1D Klein-Gordon Eqn (6.1),

$$\ddot\psi(t,\mathbf{x}) = \psi''(t,\mathbf{x}) - m^2\psi(t,\mathbf{x}), \quad \mathbf{x} \in \mathbb{R}. \tag{8.5}$$

Then $\pi = \dot\psi$ and $Q(t) = \lim_{R\to\infty} Q_R(t)$, where

$$Q_R(t) = \int_{-R}^{R} \dot\psi(t,\mathbf{x}) \cdot i\psi(t,\mathbf{x}) d\mathbf{x}. \tag{8.6}$$

Differentiating, we get

$$\dot Q_R(t) = \int_{-R}^{R} \ddot\psi(t,\mathbf{x}) \cdot i\psi(t,\mathbf{x}) d\mathbf{x} + \int_{-R}^{R} \dot\psi(t,\mathbf{x}) \cdot i\dot\psi(t,\mathbf{x}) d\mathbf{x}. \tag{8.7}$$

The second integral in the RHS is zero since $z_1 \cdot iz_2$ is an antisymmetric bilinear form in $\mathbb{C}$ by (6.4). Hence, substituting $\ddot\psi(t,\mathbf{x}) = \psi''(t,\mathbf{x}) - m^2\psi(t,\mathbf{x})$ from (8.5), we get by the partial integration,

$$\begin{aligned} \dot Q_R(t) &= \psi'(t,\mathbf{x}) \cdot i\psi(t,\mathbf{x})\Big|_{-R}^{R} - \int_{-R}^{R} \psi'(t,\mathbf{x}) \cdot i\psi'(t,\mathbf{x}) d\mathbf{x} - m^2 \int_{-R}^{R} \psi(t,\mathbf{x}) \cdot i\psi(t,\mathbf{x}) d\mathbf{x} \\ &= \psi'(t,\mathbf{x}) \cdot i\psi(t,\mathbf{x})\Big|_{-R}^{R} = j(t,-R) - j(t,R), \quad j(t,x) := -\psi'(t,\mathbf{x}) \cdot i\psi(t,\mathbf{x}). \end{aligned} \tag{8.8}$$

since both integrals are zero by the antisymmetry. Therefore, (6.18) implies that for every fixed t we have $\dot Q_R(t) \to 0$ as $R \to \infty$, hence $Q(t)$ =const. ■

Remark 8.10 *The identity (8.8) means that $j(t,x)$ is the* **charge current density** *for the 1D Klein-Gordon Eqn.*

Exercise 8.11 *Prove the Theorem 8.9 for the nonlinear 1D Schrödinger Eqn (6.2),*

$$i\dot\psi(t,\mathbf{x}) = \frac{1}{2m}\psi''(t,\mathbf{x}) + F(\psi), \quad \mathbf{x} \in \mathbb{R}, \tag{8.9}$$

where $F(\psi) = -\nabla U(|\psi|)$, $\psi \in \mathbb{C} \equiv \mathbb{R}^2$.

Exercise 8.12 *Prove the Theorem 8.9 for the general case and check the formulas for the charge current*

$$\mathbf{j}(t,x) := -\nabla_{\mathbf{x}}\psi(t,\mathbf{x}) \cdot i\psi(t,\mathbf{x}). \tag{8.10}$$

9 E.Noether Currents Theory

9.1 Field Symmetry and Noether Theorem II

Let us consider a generalization of the symmetry theory to Lagrangian fields. Consider the one-parametric group of transformations $g_s : \mathbb{R}^4 \times \mathbb{R}^N \to \mathbb{R}^4 \times \mathbb{R}^N$ of the form

$$g_s : \begin{pmatrix} x \\ \psi \end{pmatrix} \mapsto \begin{pmatrix} y \\ \psi_s \end{pmatrix} = \begin{pmatrix} a_s(x) \\ b_s(\psi) \end{pmatrix} \Big| \quad s \in \mathbb{R} \tag{9.1}$$

where a_s resp. b_s are some differentiable transformations $a_s : \mathbb{R}^4 \to \mathbb{R}^4$ resp. $b_s : \mathbb{R}^N \to \mathbb{R}^N$. Let us define the corresponding transformations of the fields

$$\psi(x) \mapsto \psi_s(y) := b_s(\psi(x)). \tag{9.2}$$

This definition implies corresponding transformation for the derivatives: by the chain rule,

$$\nabla\psi(x) \mapsto \nabla_y \psi_s(y) := \nabla_\psi b_s(\psi(x)) \nabla\psi(x) \frac{\partial x(y)}{\partial y}. \tag{9.3}$$

Remark 9.1 *At $s = 0$ all transformations are identities since $g_0 = Id$ for the* **group** *g_s (cf. (4.4)):*

$$(a_0 x, b_0 \psi) = (x, \psi), \quad (x, \psi) \in \mathbb{R}^4 \times \mathbb{R}^N. \tag{9.4}$$

Definition 9.2 *The transformation g_s, $s \in \mathbb{R}$, is a symmetry of the Lagrangian field with the Lagrangian density $\mathcal{L}(x, \psi, \nabla\psi)$ if the following identity holds,*

$$\mathcal{L}(x, \psi, \nabla\psi) = \mathcal{L}(y, \psi_s, \nabla_y \psi_s) \Big| \frac{\partial y(x)}{\partial x} \Big|, \qquad (x, \psi, \nabla\psi) \in \mathbb{R}^{d+1} \times \mathbb{R}^N \times \mathbb{R}^{(4)N}. \tag{9.5}$$

Example 9.3 Time-translations *Consider the time-translations along $e_0 = (1, 0, 0, 0)$,*

$$g_s : \begin{pmatrix} x \\ \psi \end{pmatrix} \mapsto \begin{pmatrix} y \\ \psi_s \end{pmatrix} = \begin{pmatrix} x - se_0 \\ \psi \end{pmatrix} \Big| \quad s \in \mathbb{R}. \tag{9.6}$$

Then

$$\psi_s(y) = \psi(y + se_0), \quad \nabla_y \psi_s(y) = (\nabla\psi)(y + se_0), \qquad \Big| \frac{\partial y(x)}{\partial x} \Big| \equiv 1. \tag{9.7}$$

Hence, (9.5) for the transformations is equivalent to (7.7).

Example 9.4 Space-translations *Consider the space-translations along $e_1 = (0, 1, 0, 0)$,*

$$g_s : \begin{pmatrix} x \\ \psi \end{pmatrix} \mapsto \begin{pmatrix} y \\ \psi_s \end{pmatrix} = \begin{pmatrix} x + se_1 \\ \psi \end{pmatrix} \Big| \quad s \in \mathbb{R}. \tag{9.8}$$

Then

$$\psi_s(y) = \psi(y - se_1), \quad \nabla_y \psi_s(y) = (\nabla\psi)(y - se_1), \qquad \Big| \frac{\partial y(x)}{\partial x} \Big| \equiv 1. \tag{9.9}$$

Hence, (9.5) for the transformations is equivalent to (7.17).

Example 9.5 Space-rotations *Consider the rotations,*

$$g_s: \begin{pmatrix} (x_0,\mathbf{x}) \\ \psi \end{pmatrix} \mapsto \begin{pmatrix} y \\ \psi_s \end{pmatrix} = \begin{pmatrix} (x_0, O_3(-s)\mathbf{x}) \\ \psi \end{pmatrix} \Bigg| \quad s \in \mathbb{R}, \tag{9.10}$$

where $O_3(s)$ is the rotation of $\mathbb{R}^3$ around e_3 with an angle of s radian. Then

$$\psi_s(y) = \psi(y_0, O_3(s)\mathbf{y}), \quad \nabla_y \psi_s(y) = (\nabla\psi)(y_0, O_3(s)\mathbf{y}) \begin{pmatrix} 1 & 0 \\ 0 & O_3(s) \end{pmatrix}, \quad \left|\frac{\partial y(x)}{\partial x}\right| \equiv 1. \tag{9.11}$$

Hence, (8.1) implies (9.5) for the transformations.

Example 9.6 Internal rotations *For $\psi \in \mathbb{C}^M$: consider the internal rotations,*

$$g_s: \begin{pmatrix} x \\ \psi \end{pmatrix} \mapsto \begin{pmatrix} y \\ \psi_s \end{pmatrix} = \begin{pmatrix} x \\ e^{is}\psi \end{pmatrix} \Bigg| \quad s \in \mathbb{R}. \tag{9.12}$$

Then

$$\psi_s(y) = e^{is}\psi(y), \quad \nabla_y \psi_s(y) = e^{is}\nabla\psi(y), \qquad \left|\frac{\partial y(x)}{\partial x}\right| \equiv 1. \tag{9.13}$$

Hence, (8.3) implies (9.5) for the transformations.

Definition 9.7 *For a given one-parametric group of transformations (9.1) and a given trajectory $\psi(x)$ let us define the vector fields*

$$v(x) = \frac{\partial a_s x}{\partial s}\bigg|_{s=0}, \qquad w(x) = \frac{\partial \psi_s(x)}{\partial s}\bigg|_{s=0}, \qquad x \in \mathbb{R}^{d+1}. \tag{9.14}$$

Definition 9.8 *The Noether current, $\alpha = 0, ..., 3$,*

$$S_\alpha(x) = \pi_\alpha(x) w(x) + \mathcal{L}(x, \psi(x), \nabla\psi(x)) v_\alpha(x), \qquad x \in \mathbb{R}^{d+1}. \tag{9.15}$$

Theorem 9.9 (E.Noether [11]) *Let (9.5) hold for $s \in \mathbb{R}$. Let $\psi(x) \in C^2(\mathbb{R}^4, \mathbb{R}^N)$ be a solution to the equations (6.10), and $w(x) \in C^1(\mathbb{R}^4, \mathbb{R}^N)$, $v(x) \in C^1(\mathbb{R}^4, \mathbb{R}^4)$ are defined by (9.14). Then the continuity equation holds,*

$$\partial_\alpha S_\alpha(x) = 0, \quad x \in \mathbb{R}^4. \tag{9.16}$$

Corollary 9.10 *Let all conditions of Theorem 9.9 hold and additionally, the bounds (6.20) hold and $\psi(x) \in C^2_\sigma$, $w(x) \in C^1_\sigma$ with a $\sigma > 3/2$, and $v(x) \in C^1_0$. Then the conservation law holds,*

$$\mathcal{S}_0(t) := \int_{\mathbb{R}^3} S_0(t, \mathbf{x}) d\mathbf{x} = \text{const}, \quad t \in \mathbb{R}. \tag{9.17}$$

Proof We have $\mathcal{S}(t) = \lim_{R \to]\infty} \mathcal{S}^R_0(t)$ where

$$\mathcal{S}^R_0(t) := \int_{|\mathbf{x}| \le R} S_0(t, \mathbf{x}) d\mathbf{x}, \quad t \in \mathbb{R}. \tag{9.18}$$

Differentiating, we get by (9.16) and the Stokes Theorem,

$$\dot{\mathcal{S}}^R_0(t) := -\int_{|\mathbf{x}| \le R} \nabla_k S_k(t, \mathbf{x}) d\mathbf{x} = -\int_{|\mathbf{x}| = R} n_k(\mathbf{x}) S_k(t, \mathbf{x}) d\Sigma, \quad t \in \mathbb{R}, \tag{9.19}$$

where $n_k(\mathbf{x}) := x_k/|\mathbf{x}|$ and $d\Sigma$ is the Lebesgue measure on the sphere $|\mathbf{x}| = R$. Therefore, $\dot{\mathcal{S}}^R_0(t) \to 0$ as $R \to \infty$ since $S_k(x) \in C^1_\sigma$ with $\sigma > 3$. Hence (9.17) follows. ■

Remark 9.11 *The integral identity (9.19) means that the vector field $S_k(t,\mathbf{x})$ is the current density of the field $S_0(t,\mathbf{x})$.*

Proof of Theorem 9.9 (cf. [7]) Consider an arbitrary open region $\Omega \subset \mathbb{R}^3$ with a smooth boundary. Integrating the symmetry condition (9.5) over Ω, we get

$$\int_\Omega \mathcal{L}(x,\psi(x),\nabla\psi(x))dx = \int_{\Omega_s} \mathcal{L}(y,\psi_s(y),\nabla_y\psi_s(y))dy, \qquad s\in\mathbb{R}, \tag{9.20}$$

where $\Omega_s := a_s(\Omega)$. Let us make the change of variables $y = a_s(x)$ in the RHS. Then we get the identity

$$\int_\Omega \mathcal{L}(a_s(x),b_s(\psi(x)),D_s(x))I_s(x)dx = \text{const}, \qquad s\in\mathbb{R}, \tag{9.21}$$

where $I_s(x) := \left|\dfrac{\partial a_s(x)}{\partial x}\right|$ and

$$[D_s(x)]_\alpha := \left.\frac{\partial\psi_s(y)}{\partial y_\alpha}\right|_{y=a_s(x)}, \quad \alpha = 0,...,d. \tag{9.22}$$

Differentiating (9.21) in s, we get by (9.4),

$$\int_\Omega \Big[\mathcal{L}_x(x,\psi(x),\nabla\psi(x))\cdot\left.\frac{d}{ds}\right|_{s=0} a_s(x) + \mathcal{L}_\psi(x,\psi(x),\nabla\psi(x))\cdot\left.\frac{d}{ds}\right|_{s=0} b_s(\psi(x))$$
$$+\mathcal{L}_{\nabla_\alpha\psi}(x,\psi(x),\nabla\psi(x))\cdot\left.\frac{d}{ds}\right|_{s=0}[D_s(x)]_\alpha + \mathcal{L}(x,\psi(x),\nabla\psi(x))\left.\frac{d}{ds}\right|_{s=0} I_s(\psi(x))\Big]dx = 0. \tag{9.23}$$

Let us calculate the four derivatives in s.
i) By the definition (9.14),

$$\left.\frac{d}{ds}\right|_{s=0} a_s(x) = v(x). \tag{9.24}$$

ii) By the definition (9.2), the chain rule and (9.14), (9.4),

$$\left.\frac{d}{ds}\right|_{s=0} b_s(\psi(x)) = \left.\frac{d}{ds}\right|_{s=0} \psi_s(a_s x) = \left.\frac{d}{ds}\right|_{s=0} [\psi_s(a_0 x) + \psi_0(a_s x)] = w(x) + \nabla\psi(x)\cdot v(x). \tag{9.25}$$

iii) Formally $[D_s(x)]_\alpha := \dfrac{\partial b_s(\psi(x))}{\partial[a_s(x)]_\alpha} = \dfrac{\partial\psi_s(a_s(x))}{\partial[a_s(x)]_\alpha}$. Hence the same arguments imply formally

$$\begin{aligned}
\left.\frac{d}{ds}\right|_{s=0}[D_s(x)]_\alpha &= \left.\frac{d}{ds}\right|_{s=0}\frac{\partial\psi_s(a_s(x))}{\partial[a_s(x)]_\alpha} \\
&= \left.\frac{d}{ds}\right|_{s=0}\left[\frac{\partial\psi_s(a_0(x))}{\partial[a_0(x)]_\alpha} + \frac{\partial\psi_0(a_s(x))}{\partial[a_0(x)]_\alpha} + \frac{\partial\psi_0(a_0(x))}{\partial[a_s(x)]_\alpha}\right] \\
&= \nabla_\alpha w(x) + \nabla_\alpha(\nabla\psi(x)v(x)) + \left.\frac{d}{ds}\right|_{s=0}\frac{\partial\psi(x)}{\partial[a_s(x)]_\alpha}.
\end{aligned} \tag{9.26}$$

To calculate the last derivative, let us use the matrix identity

$$\frac{\partial\psi(x)}{\partial[a_s(x)]_\beta}\frac{\partial[a_s(x)]_\beta}{\partial x_\alpha} = \frac{\partial\psi(x)}{\partial x_\alpha} \tag{9.27}$$

Differentiating in s, we get by (9.4),

$$\frac{d}{ds}\Big|_{s=0}\frac{\partial\psi(x)}{\partial[a_s(x)]_\alpha} + \frac{\partial\psi(x)}{\partial x_\beta}\frac{\partial v_\beta}{\partial x_\alpha} = 0. \tag{9.28}$$

Therefore, the last derivative in (9.26) equals $-\nabla\psi\nabla_\alpha v$. Hence (9.26) becomes,

$$\frac{d}{ds}\Big|_{s=0}[D_s(x)]_\alpha = \nabla_\alpha w(x) + \nabla(\nabla_\alpha\psi(x))\cdot v(x). \tag{9.29}$$

iv) Finally, the derivative of the determinant I_s of the Jacobian matrix is the trace of the derivative,

$$\frac{d}{ds}\Big|_{s=0} I_s(\psi(x)) = \frac{d}{ds}\Big|_{s=0}\Big|\frac{\partial a_s(x)}{\partial x}\Big| = \mathrm{tr}\frac{d}{ds}\Big|_{s=0}\frac{\partial a_s(x)}{\partial x} = \mathrm{tr}\frac{\partial v(x)}{\partial x} = \nabla\cdot v(x) \tag{9.30}$$

since the Jacobian matrix is diagonal: $\dfrac{\partial a_0(x)}{\partial x} = E$.

Collecting all calculations i) – iv) in (9.23), we get

$$\begin{aligned}&\int_\Omega\Big[\mathcal{L}_x(x,\psi(x),\nabla\psi(x))\cdot v(x) + \mathcal{L}_\psi(x,\psi(x),\nabla\psi(x))\cdot(w(x)+\nabla\psi(x)\cdot v(x))\\ &+\pi_\alpha(x)\cdot(\nabla_\alpha w(x) + \nabla(\nabla_\alpha\psi(x))\cdot v(x))\\ &+\mathcal{L}(x,\psi(x),\nabla\psi(x))\nabla\cdot v(x)\Big]dx = 0.\end{aligned} \tag{9.31}$$

Since the region Ω is arbitrary, the integrand is zero by the Main Lemma of Calculus of Variations. We rewrite it as follows,

$$\mathcal{L}_\psi\cdot w(x) + \pi_\alpha(x)\cdot\nabla_\alpha w(x) + \nabla\cdot\Big[\mathcal{L}(x,\psi(x),\nabla\psi(x))v(x)\Big] = 0. \tag{9.32}$$

Finally let us substitute $\mathcal{L}_\psi = \nabla_\alpha\pi_\alpha(x)$ from the Euler-Lagrange Equations (6.10). Then (9.32) becomes,

$$\nabla_\alpha\Big[\pi_\alpha(x)\cdot w(x)\Big] + \nabla\cdot\Big[\mathcal{L}(x,\psi(x),\nabla\psi(x))v(x)\Big] = 0 \tag{9.33}$$

which coincides with (9.16) by (9.15). ■

Remark 9.12 *The justification of the formal proof (9.26) – (9.28) of (9.29) follows from the identity of type (9.27),*

$$[D_s(x)]_\beta\frac{\partial[a_s(x)]_\beta}{\partial x_\alpha} = \frac{\partial\psi(a_s x)}{\partial x_\alpha} \tag{9.34}$$

by differentiation similar to (9.28) and (9.26).

10 Applications of the Noether Theorem

10.1 Four Conservation Laws for Classical Wave Fields

Let us apply the Noether Theorem to the four groups of the examples 9.3 – 9.6.

I. Proof of Theorem 7.4 For the group (9.6) the definition (9.14) implies by (9.7),

$$v(x) = -e_0, \qquad w(x) = \nabla\psi(x)e_0 = \nabla_0\psi(x), \qquad x \in \mathbb{R}^4. \tag{10.1}$$

Hence, the Noether current (9.15) becomes,

$$\begin{cases} S_0(x) &= \pi_0(x)\nabla_0\psi(x) - \mathcal{L}(x, \psi(x), \nabla\psi(x)), \\ S_k(x) &= \pi_k(x)\nabla_0\psi(x), \quad k = 1, 2, 3. \end{cases} \tag{10.2}$$

The identity (7.7) implies that the Lagrangian density satisfies the invariance condition (9.5) with the group (9.6). Therefore, Theorem 9.9 implies the continuity equation (9.16) for the current (10.2), and Corollary 9.10 implies (9.17) which means the energy conservation by Definition (7.1).

II. Proof of Theorem 7.7 For the group (9.8) the definition (9.14) implies by (9.9),

$$v(x) = e_1, \qquad w(x) = -\nabla\psi(x)e_1 = -\nabla_1\psi(x), \qquad x \in \mathbb{R}^4. \tag{10.3}$$

Hence, the Noether current (9.15) becomes,

$$\begin{cases} S_0(x) &= -\pi_0(x)\nabla_1\psi(x), \\ S_1(x) &= -\pi_1(x)\nabla_1\psi(x) + \mathcal{L}(x, \psi(x), \nabla\psi(x)), \\ S_k(x) &= -\pi_k(x)\nabla_1\psi(x), \quad k = 2, 3. \end{cases} \tag{10.4}$$

The identity (7.17) implies that the Lagrangian density satisfies the invariance condition (9.5) with the group (9.8). Therefore, Theorem 9.9 implies the continuity equation (9.16) for the current (10.4), and Corollary 9.10 implies (9.17) which means the conservation of the first component of the momentum by Definition (7.2).

III. Proof of Theorem 8.3 For the group (9.10) the definition (9.14) implies by (9.11) and (2.31),

$$v(x) = (0, e_3 \times \mathbf{x}), \;\; w(x) = \nabla\psi(x)(0, e_3 \times \mathbf{x}) = (\mathbf{x} \times \nabla_{\mathbf{x}})_3\psi(x), \quad x \in \mathbb{R}^4. \tag{10.5}$$

Hence, the Noether current (9.15) becomes,

$$\begin{cases} S_0(x) &= \pi_0(x)(\mathbf{x} \times \nabla_{\mathbf{x}})_3\psi(x), \\ S_k(x) &= \pi_k(x)(\mathbf{x} \times \nabla_{\mathbf{x}})_3\psi(x) + \mathcal{L}e_3 \times \mathbf{x}, \quad k = 1, 2, 3. \end{cases} \tag{10.6}$$

The identity (8.1) implies that the Lagrangian density satisfies the invariance condition (9.5) with the group (9.10). Therefore, Theorem 9.9 implies the continuity equation (9.16) for the current (10.6), and Corollary 9.10 implies (9.17) which means the conservation of the third component of the angular momentum by Definition (8.2).

IV. Proof of Theorem 8.9 For the group (9.12) the definition (9.14) implies by (9.13),

$$v(x) = 0, \;\; w(x) = i\psi(x), \quad x \in \mathbb{R}^4. \tag{10.7}$$

Hence, the Noether current (9.15) becomes the charge-current densities,

$$S_\alpha(x) = \pi_\alpha(x) \cdot i\psi(x), \qquad \alpha = 0, ..., 3. \tag{10.8}$$

The identity (8.3) implies that the Lagrangian density satisfies the invariance condition (9.5) with the group (9.12). Therefore, Theorem 9.9 implies the continuity equation (9.16) for the current (10.8), and Corollary 9.10 implies (9.17) which means the charge conservation by Definition (8.4).

10.2 Nonlinear Klein-Gordon Eqn

Let us substitute the expressions (6.16) and (6.6) into (10.2), (10.4), (10.6) and (10.8). Then Theorem 9.9 implies for solutions to the equation (6.1):
I. Energy flux The continuity equation (9.16) holds for the energy- and energy current densities

$$
\left\{\begin{array}{rcl}
S_0(x) &=& -i\hbar(i\hbar\nabla_0 - \not{\phi}(x))\psi(x)\cdot\nabla_0\psi(x) - \mathcal{L}(x,\psi(x),\nabla\psi(x)) \\
&=& \dfrac{(i\hbar\nabla_0 - \not{\phi}(x))\psi(x)\cdot(i\hbar\nabla_0 + \not{\phi}(x))\psi(x)}{2}, \\
&& + \sum\limits_{k=1}^{3}\dfrac{|(-i\hbar\nabla_k - \not{A}_k(x))\psi(x)|^2}{2}, \\
S_k(x) &=& -i\hbar(-i\hbar\nabla_k - \not{A}_k(x))\psi(x)\cdot\nabla_0\psi(x), \quad k=1,2,3.
\end{array}\right. \tag{10.9}
$$

if the potentials $\phi(x), A(x)$ do not depend on time $x_0 = ct$.
For free linear equation (6.11):

$$
\left\{\begin{array}{rcl}
S_0(x) &=& \dfrac{|\nabla_0\psi(x)|^2}{2} + \sum\limits_{k=1}^{3}\dfrac{|\nabla_k\psi(x)|^2}{2} + m^2\dfrac{|\psi(x)|^2}{2}, \\
S_k(x) &=& -\nabla_k\psi(x)\cdot\nabla_0\psi(x), \quad k=1,2,3.
\end{array}\right. \tag{10.10}
$$

II. Momentum flux The continuity equation (9.16) holds for the first components of the momentum- and momentum current densities

$$
\left\{\begin{array}{rcl}
S_0(x) &=& i\hbar(i\hbar\nabla_0 - \not{\phi}(x))\psi(x)\cdot\nabla_1\psi(x), \\
S_1(x) &=& i\hbar(-i\hbar\nabla_1 - \not{A}_1(x))\psi(x)\cdot\nabla_1\psi(x) + \mathcal{L}(x,\psi(x),\nabla\psi(x)) \\
&=& \dfrac{|(-i\hbar\nabla_0 - \not{\phi}(x))\psi(x)|^2}{2} + \dfrac{(-i\hbar\nabla_1 - \not{A}_1(x))\psi(x)\cdot(-i\hbar\nabla_1 + \not{A}_1(x))\psi(x)}{2} \\
&& + \sum\limits_{k=2}^{3}\dfrac{|(-i\hbar\nabla_k - \not{A}_k(x))\psi(x)|^2}{2}, \\
S_k(x) &=& i\hbar(-i\hbar\nabla_k - \not{A}_k(x))\psi(x)\cdot\nabla_1\psi(x), \quad k=2,3.
\end{array}\right. \tag{10.11}
$$

if the potentials $\phi(x), A(x)$ do not depend on x_1.
For free linear equation (6.11):

$$
\left\{\begin{array}{rcl}
S_0(x) &=& -\nabla_0\psi(x)\cdot\nabla_1\psi(x), \\
S_1(x) &=& \dfrac{|\nabla_0\psi(x)|^2}{2} + \dfrac{|\nabla_1\psi(x)|^2}{2} - \sum\limits_{k=2,3}\dfrac{|\nabla_k\psi(x)|^2}{2} - m^2\dfrac{|\psi(x)|^2}{2}, \\
S_k(x) &=& \nabla_k\psi(x)\cdot\nabla_1\psi(x), \quad k=2,3.
\end{array}\right. \tag{10.12}
$$

III. Space-rotations The continuity equation (9.16) holds for the third components of the angular momentum- and angular momentum current densities

$$(10.13)\quad \begin{cases} S_0(x) &= -i\hbar(i\hbar\nabla_0 - \not{\phi}(x))\psi(x)\cdot(\mathbf{x}\times\nabla_{\mathbf{x}})_3\psi(x), \\ S_k(x) &= -i\hbar(-i\hbar\nabla_k - \not{A}_k(x))\psi(x)\cdot(\mathbf{x}\times\nabla_{\mathbf{x}})_3\psi(x) + \mathcal{L}(e_3\times\mathbf{x})_k, \quad k=1,2,3 \end{cases}$$

if (8.1) holds for the density (6.6).
For free linear equation (6.11):

$$(10.14)\quad \begin{cases} S_0(x) &= \nabla_0\psi(x)(\mathbf{x}\times\nabla_{\mathbf{x}})_3\psi(x), \\ S_k(x) &= -\nabla_k\psi(x)\cdot(\mathbf{x}\times\nabla_{\mathbf{x}})_3\psi(x) + \mathcal{L}(e_3\times\mathbf{x})_k, \quad k=1,2,3. \end{cases}$$

IV. Internal rotations The continuity equation (9.16) holds for the charge- and charge current densities

$$(10.15)\quad \begin{cases} S_0(x) &= -i\hbar(i\hbar\nabla_0 - \not{\phi}(x))\psi(x)\cdot i\psi(x), \\ S_k(x) &= -i\hbar(-i\hbar\nabla_k - \not{A}_k(x))\psi(x)\cdot i\psi(x) \quad k=1,2,3 \end{cases}$$

if the "nonlinear" potential energy $U(\psi)$ depends only on $|\psi|$.
For free linear equation (6.11):

$$(10.16)\qquad S_0(x) = \nabla_0\psi(x)\cdot i\psi(x), \quad S_k(x) = -\nabla_k\psi(x)\cdot i\psi(x) \quad k=1,2,3.$$

10.3 Nonlinear Schrödinger Eqn

Let us substitute the expressions (6.17) and (6.7) into (10.2), (10.4), (10.6) and (10.8). Then Theorem 9.9 implies for solutions to the equation (6.2):
I. Energy flux The continuity equation (9.16) holds for the energy- and energy current densities

$$(10.17)\quad \begin{cases} S_0(x) &= -\dfrac{i\hbar\psi(x)}{2}\cdot\nabla_0\psi(x) - \mathcal{L}(x,\psi(x),\nabla\psi(x)) \\ &= \dfrac{e\phi(x)\psi(x)\cdot\psi(x)}{2} + \dfrac{1}{2m}\displaystyle\sum_{k=1}^{3}\frac{|(-i\hbar\nabla_k - \not{A}_k(x))\psi(x)|^2}{2} \\ S_k(x) &= -\dfrac{1}{2m}i\hbar(-i\hbar\nabla_k - \not{A}_k(x))\psi(x)\cdot\nabla_0\psi(x), \quad k=1,2,3 \end{cases}$$

if the potentials $\phi(x), A(x)$ do not depend on time $x_0 = ct$.
For free linear equation (6.11):

$$(10.18)\quad \begin{cases} S_0(x) &= \dfrac{1}{2m}\displaystyle\sum_{k=1}^{3}\frac{|\nabla_k\psi(x)|^2}{2}, \\ S_k(x) &= -\dfrac{1}{2m}\nabla_k\psi(x)\cdot\nabla_0\psi(x), \quad k=1,2,3. \end{cases}$$

II. Momentum flux The continuity equation (9.16) holds for the first components of the momentum- and momentum current densities

$$
(10.19)\quad \begin{cases} S_0(x) = \dfrac{i\hbar\psi(x)}{2}\cdot\nabla_1\psi(x), \\ S_1(x) = \dfrac{1}{2m}i\hbar(-i\hbar\nabla_1 - \not{e}A_1(x))\psi(x)\cdot\nabla_1\psi(x) + \mathcal{L}(x,\psi(x),\nabla\psi(x)) \\ \qquad = \dfrac{e\phi(x)\psi(x)\cdot\psi(x)}{2} + \dfrac{1}{2m}\dfrac{(-i\hbar\nabla_1 - \not{e}A_1(x))\psi(x)\cdot(-i\hbar\nabla_1 + \not{e}A_1(x))\psi(x)}{2} \\ \qquad\quad -\dfrac{1}{2m}\sum_{k=2}^{3}\dfrac{|(-i\hbar\nabla_k - \not{e}A_k(x))\psi(x)|^2}{2}, \\ S_k(x) = \dfrac{1}{2m}i\hbar(-i\hbar\nabla_k - \not{e}A_k(x))\psi(x)\cdot\nabla_1\psi(x), \quad k=2,3 \end{cases}
$$

if the potentials $\phi(x), A(x)$ do not depend on x_1.
For free linear equation (6.11):

$$
(10.20)\quad \begin{cases} S_0(x) = \dfrac{i\psi(x)}{2}\cdot\nabla_1(x), \\ S_1(x) = -\dfrac{i\nabla_0(x)\cdot\psi(x)}{2} + \dfrac{1}{2m}\dfrac{|\nabla_1\psi(x)|^2}{2} - \dfrac{1}{2m}\sum_{k=2,3}\dfrac{|\nabla_k\psi(x)|^2}{2}, \\ S_k(x) = \dfrac{1}{2m}\nabla_k\psi(x)\cdot\nabla_1\psi(x), \quad k=2,3. \end{cases}
$$

III. Space-rotations The continuity equation (9.16) holds for the third components of the angular momentum- and angular momentum current densities

$$
(10.21)\quad \begin{cases} S_0(x) = -\dfrac{i\hbar\psi(x)}{2}\cdot(\mathbf{x}\times\nabla_{\mathbf{x}})_3\psi(x), \\ S_k(x) = -\dfrac{1}{2m}i\hbar(-i\hbar\nabla_k - \not{e}A_k(x))\psi(x)\cdot(\mathbf{x}\times\nabla_{\mathbf{x}})_3\psi(x) + \mathcal{L}(e_3\times\mathbf{x})_k, \quad k=1,2,3 \end{cases}
$$

if (8.1) holds for the density (6.7).
For free linear equation (6.11):

$$
(10.22)\quad \begin{cases} S_0(x) = -\dfrac{i\psi(x)}{2}\cdot(\mathbf{x}\times\nabla_{\mathbf{x}})_3\psi(x), \\ S_k(x) = -\dfrac{1}{2m}\nabla_k\psi(x)\cdot(\mathbf{x}\times\nabla_{\mathbf{x}})_3\psi(x) + \mathcal{L}(e_3\times\mathbf{x})_k, \quad k=1,2,3. \end{cases}
$$

IV. Internal rotations The continuity equation (9.16) holds for the charge- and charge current densities

$$
(10.23)\quad S_0(x) = -\frac{\hbar\psi(x)}{2}\cdot\psi(x), \quad S_k(x) = \frac{1}{2m}\hbar(i\hbar\nabla_k + \not{e}A_k(x))\psi(x)\cdot\psi(x) \quad k=1,2,3
$$

if the "nonlinear" potential energy $U(\psi)$ is a function of $|\psi|$.
For free linear equation (6.11):

$$S_0(x) = -\frac{\psi(x)}{2} \cdot \psi(x), \quad S_k(x) = \frac{1}{2m}\, i\nabla_k \psi(x) \cdot \psi(x) \quad k = 1, 2, 3. \tag{10.24}$$

11 Maxwell Field

11.1 3D Electromagnetic Fields and Potentials

In 1862 Maxwell completed the Coulomb, Faraday and Biot-Savart-Laplace equations by the *displacement current* and wrote the complete system of *Classical Electrodynamics*. In *Gaussian units* it reads,

$$(11.1)\quad \left\{\begin{array}{ll} \text{div } E(t,\mathbf{x}) = 4\pi\rho(t,\mathbf{x}), & \text{rot } E(t,\mathbf{x}) = -\frac{1}{c}\dot{B}(t,\mathbf{x}), \\ \text{div } B(t,\mathbf{x}) = 0, & \text{rot } B(t,\mathbf{x}) = \frac{1}{c}\dot{E}(t,\mathbf{x}) + \frac{4\pi}{c}\mathbf{j}(t,\mathbf{x}), \end{array}\right| \qquad (t,\mathbf{x}) \in \mathbb{R}^4.$$

where $\rho(t,\mathbf{x})$ resp $\mathbf{j}(t,\mathbf{x})$ stands for the charge resp. current density.

Remark 11.1 *The Maxwell Equations imply the charge continuity equation,*

$$(11.2)\qquad \dot{\rho}(t,\mathbf{x}) + \text{div } \mathbf{j}(t,\mathbf{x}) = 0, \quad (t,\mathbf{x}) \in \mathbb{R}^4.$$

Let us introduce scalar and vector potentials to rewrite (11.1) in a relativistic covariant four-dimensional form. Namely, div $B(t,\mathbf{x}) = 0$ implies that $B(t,\mathbf{x}) = \text{rot } A(t,\mathbf{x})$. Then rot $E(t,\mathbf{x}) = -\frac{1}{c}\dot{B}(t,\mathbf{x})$ implies rot $[E(t,\mathbf{x}) + \frac{1}{c}\dot{A}(t,\mathbf{x})] = 0$ hence $E(t,\mathbf{x}) + \frac{1}{c}\dot{A}(t,\mathbf{x}) = -\nabla_{\mathbf{x}}\phi(t,\mathbf{x})$. Finally,

$$(11.3)\qquad B(t,\mathbf{x}) = \text{rot } A(t,\mathbf{x}), \quad E(t,\mathbf{x}) = -\nabla_{\mathbf{x}}\phi(t,\mathbf{x}) - \frac{1}{c}\dot{A}(t,\mathbf{x}), \qquad (t,\mathbf{x}) \in \mathbb{R}^4.$$

The justification of all the relations follows from the Fourier transform. The choice of the potentials is not unique since the *gauge transformation*

$$(11.4)\qquad \phi(t,\mathbf{x}) \mapsto \phi(t,\mathbf{x}) + \frac{1}{c}\dot{\chi}(t,\mathbf{x}), \quad A(t,\mathbf{x}) \mapsto A(t,\mathbf{x}) - \nabla_{\mathbf{x}}\chi(t,\mathbf{x})$$

does not change the fields $E(t,\mathbf{x})$, $B(t,\mathbf{x})$ for any function $\chi(t,\mathbf{x}) \in C^1(\mathbb{R}^4)$. Therefore, it is possible to satisfy an additional *gauge* condition. Let us choose for example the *Lorentz gauge*

$$(11.5)\qquad \frac{1}{c}\dot{\phi}(t,\mathbf{x}) + \text{div } A(t,\mathbf{x}) = 0, \quad (t,\mathbf{x}) \in \mathbb{R}^4.$$

Let us express the Maxwell Equations (11.1) in the potentials. Substitution of (11.3) into the first Maxwell Equation gives $4\pi\rho(t,\mathbf{x}) = \text{div } E(t,\mathbf{x}) = -\frac{1}{c}\text{div } \dot{A}(t,\mathbf{x}) - \Delta\phi(t,\mathbf{x})$. Eliminating div $\dot{A}(t,\mathbf{x})$ by the differentiation of (11.5) in time, $\frac{1}{c}\ddot{\phi}(t,\mathbf{x}) + \text{div } \dot{A}(t,\mathbf{x}) = 0$, we get

$$(11.6)\qquad \Box\phi(t,\mathbf{x}) := [\frac{1}{c^2}\partial_t^2 - \Delta]\phi(t,\mathbf{x}) = 4\pi\rho(t,\mathbf{x}), \quad (t,\mathbf{x}) \in \mathbb{R}^4.$$

Similarly, substituting (11.3) into the last Maxwell Equation, we get

$$(11.7)\quad \text{rot rot } A(t,\mathbf{x}) = \frac{1}{c}\dot{E}(t,\mathbf{x}) + \frac{4\pi}{c}\mathbf{j}(t,\mathbf{x}) = -\frac{1}{c^2}\ddot{A}(t,\mathbf{x}) - \frac{1}{c}\nabla_{\mathbf{x}}\dot{\phi}(t,\mathbf{x}) + \frac{4\pi}{c}\mathbf{j}(t,\mathbf{x}).$$

Example 11.2 *Prove the identity*

$$(11.8)\qquad \text{rot rot } = -\Delta + \nabla_{\mathbf{x}}\text{div}$$

Substituting (11.8) into (11.7) and eliminating $\frac{1}{c}\nabla_{\mathbf{x}}\dot{\phi}(t,\mathbf{x})$ by application of $\nabla_{\mathbf{x}}$ to (11.5), we get

$$\Box A(t,\mathbf{x}) = \frac{4\pi}{c}\mathbf{j}(t,\mathbf{x}), \quad (t,\mathbf{x}) \in \mathbb{R}^4. \tag{11.9}$$

Remark 11.3 *The arguments above show that the Maxwell Equations (11.1) are equivalent to the system of two wave equations (11.6), (11.9) for the potentials with the Lorentz gauge condition (11.5).*

11.2 Light and relativity

The wave equations (11.6) and (11.9) have been found by Maxwell in 1864 and led to the following two great discoveries of Maxwell and Einstein respectively:

I. The electromagnetic nature of the light Let us note that Maxwell derived the equations from the system (11.1) written in the MKS system of units:

$$\left\{\begin{array}{ll} \text{div } E(t,\mathbf{x}) = \frac{4\pi}{\varepsilon_0}\rho(t,\mathbf{x}), & \text{rot } E(t,\mathbf{x}) = -\dot{B}(t,\mathbf{x}), \\ \text{div } B(t,\mathbf{x}) = 0, & \text{rot } B(t,\mathbf{x}) = \mu_0[\dot{E}(t,\mathbf{x}) + 4\pi\mathbf{j}(t,\mathbf{x})], \end{array}\right. \quad (t,\mathbf{x}) \in \mathbb{R}^4. \tag{11.10}$$

The equations contain the dielectric permittivity and magnetic permeability of the vacuum, ε_0 and μ_0, and do not contain the speed of light c. Maxwell deduced (11.6) and (11.9) with the coefficient $1/(\varepsilon_0\mu_0)$ instead of c^2 and calculated the value $1/\sqrt{\varepsilon_0\mu_0}$ since it was known that this value is the spread velocity for the wave equation. He discovered that $1/\sqrt{\varepsilon_0\mu_0}$ is very close to the speed of light c. Furthermore, he found that the electromagnetic waves are transversal like the light waves. This is why Maxwell suggested to identify the electromagnetic waves with the light.

II. The Relativity Theory The discovery of Maxwell led to a new very difficult question. The spread velocity can be equal to c only in a **unique distinguished frame of reference**: in other frames the velocity is the sum of c and a vector of the relative velocity of the frame of reference. This is why Michelson and Morley started around 1880 the famous experiment to check that the spread velocity depends on the frame of reference. They compared the wavelengths of the light along and against the velocity of the Earth motion around the Sun. However, the result was negative and very discouraging: the wave lengths were identical, hence the spread velocity does not depend on the frame of reference! Astronomical observations of *double stars* by de Sitter (1908) confirmed the negative result of Michelson and Morley. Also the experiment of Trouton and Noble confirmed the negative result.

Various partial explanations of the negative results were proposed by Ritz, Fitzgerald, Lorentz and others. The complete explanation has been provided in 1905 by Einstein who was able to cumulate the Maxwell and Lorentz ideas into a new complete theory. The main novelty was the following postulate of the Einstein theory:

the time in a moving frame is distinct from the time in the rest frame!
Namely, the transformation of space-time coordinates from the rest frame to the moving frame

of reference is given by the **Lorentz transformation**

$$\left\{\begin{array}{rcccl} t & \mapsto & t' & = & \dfrac{t-\frac{v}{c^2}x_1}{\sqrt{1-\beta^2}} \\ x_1 & \mapsto & x_1' & = & \dfrac{x_1-vt}{\sqrt{1-\beta^2}} \\ x_2 & \mapsto & x_2' & = & x_2 \\ x_3 & \mapsto & x_3' & = & x_3 \end{array}\right. \tag{11.11}$$

where (t, x_1, x_2, x_3) stands for the time-space coordinates in the rest frame and (t', x_1', x_2', x_3') corresponds to the moving frame if the relative velocity is $(v, 0, 0)$, $|v| < c$ and $\beta := v/c$.

Exercise 11.4 *Check that the wave equation*

$$\Box\psi(t,\mathbf{x}) := (\frac{1}{c^2}\,\partial_t - \Delta)\psi(t,\mathbf{x}) = 0, \quad (t,\mathbf{x}) \in \mathbb{R}^4 \tag{11.12}$$

is invariant with respect to the transformations (11.11).
Hints: *i) Set $c = 1$ and use that $\partial_2 = \partial_2'$, $\partial_3 = \partial_3'$. ii) Check that the 1D equation $(\partial_t^2 - \partial_1^2)\psi(t,x) = 0$, $(t,x) \in \mathbb{R}^2$ is equivalent to $[(\partial_t')^2 - (\partial_1')^2)]\psi(t,x) = 0$ where $t' = at - bx$ and $x' = ax - bt$, and $a^2 - b^2 = 1$.*

Exercise 11.5 *Check that the wave equations (11.6) and (11.9) are* **not** *invariant with respect to the standard* **Galilean transformation**

$$\left\{\begin{array}{rcccl} t & \mapsto & t' & = & t \\ x_1 & \mapsto & x_1' & = & x_1 - vt \\ x_2 & \mapsto & x_2' & = & x_2 \\ x_3 & \mapsto & x_3' & = & x_3 \end{array}\right. \tag{11.13}$$

12 Dynamics of Maxwell Field

Let us state in an appropriate form a convolution representation for solutions to Maxwell Eqns (11.1). Let us consider the Cauchy problem for the equations with the initial conditions

$$E|_{t=0} = E_0(\mathbf{x}), \quad B|_{t=0} = B_0(\mathbf{x}), \qquad \mathbf{x} \in \mathbb{R}^3. \tag{12.1}$$

We assume $(E_0(\mathbf{x}), B_0(\mathbf{x})) \in L^2 \oplus L^2$, where $L^2 = L^2(\mathbb{R}^3) \otimes \mathbb{R}^3$, $\rho(t,\mathbf{x}) \in C(\mathbb{R}, L^2(\mathbb{R}^3))$, $\mathbf{j}(t,\mathbf{x}) \in C(\mathbb{R}, L^2)$ and also $(E(t,\mathbf{x}), B(t,\mathbf{x})) \in C(\mathbb{R}, L^2 \oplus L^2)$. Then the system (11.1) leads to the identities

$$\text{div } E_0(\mathbf{x}) = 4\pi\rho(\mathbf{x},0) \qquad \text{div } B_0(\mathbf{x}) = 0, \quad \mathbf{x} \in \mathbb{R}^3, \tag{12.2}$$

which are necessary constraints for the existence of solutions to the overdetermined system (11.1).

Theorem 12.1 *Let $E_0(x), B_0(x)$ and $\rho(t,\mathbf{x}), \mathbf{j}(t,\mathbf{x})$ satisfy all conditions mentioned above and the constraints (11.2) and (12.2). Then*
i) The Cauchy problem (11.1), (12.1) has a unique solution $(E(t,\mathbf{x}), B(t,\mathbf{x})) \in C(\mathbb{R}, L^2 \oplus L^2)$.
ii) Let $\mathbf{j}(t,\mathbf{x}) \equiv 0$. Then the energy is conserved:

$$\int_{\mathbb{R}^3} [E^2(t,\mathbf{x}) + B^2(t,\mathbf{x})] d\mathbf{x} = \text{const}, \qquad t \in \mathbb{R}^3. \tag{12.3}$$

iii) The convolution representation holds

$$\begin{pmatrix} E(t) \\ B(t) \end{pmatrix} = \mathcal{M}_t * \begin{pmatrix} E_0 \\ B_0 \end{pmatrix} + 4\pi \int_0^t g_{t-s} * \begin{pmatrix} \rho(s) \\ \frac{1}{c}\mathbf{j}(s) \end{pmatrix} ds, \quad t \in \mathbb{R}, \tag{12.4}$$

where $E(t) := E(t,\cdot)$ etc, and $\mathcal{M}_t$ resp. g_t is 6×6- resp. 6×4- matrix valued distribution concentrated on the sphere $|\mathbf{x}| = |t|$,

$$\mathcal{M}_t(\mathbf{x}) = 0, \quad g_t(\mathbf{x}) = 0, \qquad \text{for } |\mathbf{x}| \neq |t|. \tag{12.5}$$

Proof *ad i)* We introduce the complex field $C(t,\mathbf{x}) = E(t,\mathbf{x}) + iB(t,\mathbf{x})$ and rewrite (11.1) as

$$\frac{1}{c}\dot{C}(t,\mathbf{x}) = -i \,\text{rot}\; C(t,\mathbf{x}) - \frac{4\pi}{c}\mathbf{j}(t,\mathbf{x}), \;\; C|_{t=0} = C_0(\mathbf{x}), \tag{12.6}$$

$$\text{div } C(t,\mathbf{x}) = 4\pi\rho(t,\mathbf{x}), \tag{12.7}$$

where $C_0(\mathbf{x}) = E_0(\mathbf{x}) + iB_0(\mathbf{x})$. Fourier transform $\hat{C}(\mathbf{k},t) = \int \exp(i\mathbf{k}\cdot x) C(t,\mathbf{x}) d\mathbf{x}$ leads to the equations

$$\dot{\hat{C}}(t,\mathbf{k}) = c\mathcal{M}(\mathbf{k})\hat{C}(t,\mathbf{k}) - 4\pi\hat{\mathbf{j}}(t,\mathbf{k}), \;\; \hat{C}|_{t=0} = \hat{C}_0(\mathbf{k}), \tag{12.8}$$

$$-i\mathbf{k}\cdot\hat{C}(\mathbf{k},t) = 4\pi\hat{\rho}(\mathbf{k},t), \tag{12.9}$$

where $\mathcal{M}(\mathbf{k})$ denotes the 3×3 skew-adjoint matrix of the operator $-\mathbf{k}\times$ in $\mathbb{C}^3$. The solution $\hat{C}(t,\mathbf{k})$ is defined uniquely from the first equation (12.8) of the overdetermined system (12.8), (12.9),

$$\hat{C}(t,\mathbf{k}) = \exp(c\mathcal{M}(\mathbf{k})t)\hat{C}_0(k) - 4\pi \int_0^t \exp(c\mathcal{M}(\mathbf{k})(t-s))\hat{\mathbf{j}}(s,\mathbf{k}) ds, \qquad \mathbf{k} \in \mathbb{R}^3. \tag{12.10}$$

We still have to show that (12.10) satisfies the constraints (12.9). Indeed, the Fourier transformed equations (12.2), (11.2) are

$$-i\mathbf{k}\cdot\hat{C}_0(\mathbf{k}) = 4\pi\hat{\rho}(\mathbf{k},0), \qquad \mathbf{k}\in\mathbb{R}^3, \tag{12.11}$$

$$\dot{\hat{\rho}}(t,\mathbf{k}) - ik\cdot\hat{\mathbf{j}}(t,\mathbf{k}) = 0, \qquad \mathbf{k}\in\mathbb{R}^3,\ t\in\mathbb{R}. \tag{12.12}$$

With $S(t,\mathbf{k}) = 4\pi\hat{\rho}(t,\mathbf{k}) + i\mathbf{k}\cdot\hat{C}(t,\mathbf{k})$ they imply by (12.8)

$$S(\mathbf{k},0)=4\pi\hat{\rho}(\mathbf{k},0)+i\mathbf{k}\cdot\hat{C}_0(\mathbf{k})=0, \quad \dot{S}(t,\mathbf{k})=4\pi\dot{\hat{\rho}}(t,\mathbf{k})-4\pi i\mathbf{k}\cdot\hat{\mathbf{j}}(t,\mathbf{k})=0, \quad \mathbf{k}\in\mathbb{R}^3. \tag{12.13}$$

since $k\cdot\mathcal{M}(\mathbf{k})\hat{C}(t,\mathbf{k}) = 0$. Therefore, $S(t,\mathbf{k}) = 0$ which means (12.9). Since $\mathcal{M}(\mathbf{k})$ is a skew-adjoint matrix, its exponent $\exp(c\mathcal{M}(\mathbf{k})t)$ is the unitary one. Now i) follows from (12.10).

ad ii) The Parseval identity implies that

$$\int_{\mathbb{R}^3}[E^2(t,\mathbf{x}) + B^2(t,\mathbf{x})]d\mathbf{x} = \int_{\mathbb{R}^3}|C(t,\mathbf{x})|^2 d\mathbf{x} = (2\pi)^{-3}\int_{\mathbb{R}^3}|\hat{C}(t,\mathbf{k})|^2 d\mathbf{k}. \tag{12.14}$$

Therefore, (12.3) follows from (12.10) since $\mathbf{j}(t,\mathbf{k})\equiv 0$ and $\exp(c\mathcal{M}(\mathbf{k})t)$ is the unitary matrix.

ad iii) We have to transform (12.10) back to position space in order to check (12.5). We have $\mathcal{M} = \mathcal{M}(\mathbf{k}) = -\mathbf{k}\times$, $\mathcal{M}^2 = -\mathbf{k}^2 + |\mathbf{k}><\mathbf{k}|$, $\mathcal{M}^3 = -|\mathbf{k}|^2\mathcal{M}, \ldots$. Hence

$$\mathcal{M}^{2j+1} = (-1)^j|\mathbf{k}|^{2j}\mathcal{M} = (-1)^j\frac{\mathcal{M}}{|\mathbf{k}|}|\mathbf{k}|^{2j+1} \text{ for } j\geq 0,$$

$$\mathcal{M}^{2j} = \mathcal{M}^{2j-1}\mathcal{M} = (-1)^{j-1}|\mathbf{k}|^{2j-2}\mathcal{M}^2 = -(-1)^j\left(\frac{\mathcal{M}}{|\mathbf{k}|}\right)^2|\mathbf{k}|^{2j}, \qquad j\geq 1,$$

which yields by Euler's trick for the exponential

$$\exp(\mathcal{M}(\mathbf{k})\tau) = \sum_0^\infty(\mathcal{M}\tau)^n/n! = \sum_0^\infty(\mathcal{M}\tau)^{2j}/(2j)! + \sum_0^\infty(\mathcal{M}\tau)^{2j+1}/(2j+1)! \tag{12.15}$$

$$= 1 + \left(\frac{\mathcal{M}}{|\mathbf{k}|}\right)^2(1-\cos|\mathbf{k}|\tau) + \frac{\mathcal{M}}{|\mathbf{k}|}\sin|\mathbf{k}|\tau = \cos|\mathbf{k}|\tau + \mathcal{M}\frac{\sin|\mathbf{k}|\tau}{|\mathbf{k}|} + (1-\cos|\mathbf{k}|\tau)\frac{|\mathbf{k}><\mathbf{k}|}{|\mathbf{k}|^2}.$$

Let us denote by $'$ the derivative in τ and $\hat{K}_\tau(\mathbf{k}) = \sin|\mathbf{k}|\tau/|\mathbf{k}|$, $\hat{\mathcal{M}}_\tau(\mathbf{k}) = \hat{K}'_\tau(\mathbf{k}) + \mathcal{M}\hat{K}_\tau(\mathbf{k})$, $\hat{D}_\tau(\mathbf{k}) = 1-\cos|\mathbf{k}|\tau$. Then we obtain finally,

$$\exp(\mathcal{M}(\mathbf{k})\tau) = \hat{\mathcal{M}}_\tau(\mathbf{k}) + |\mathbf{k}>\frac{\hat{D}_\tau(\mathbf{k})}{|\mathbf{k}|^2}<\mathbf{k}|. \tag{12.16}$$

Inserting into (12.10) and using the constraints (12.11) and (12.12)

$$\hat{C}(t,\mathbf{k}) = \hat{\mathcal{M}}_{ct}(\mathbf{k})\hat{C}_0(\mathbf{k}) + 4\pi i|\mathbf{k}>\frac{\hat{D}_{ct}(\mathbf{k})}{|\mathbf{k}|^2}\hat{\rho}(\mathbf{k},0) \tag{12.17}$$

$$-4\pi\int_0^t[\hat{\mathcal{M}}_{c(t-s)}(\mathbf{k})\hat{\mathbf{j}}(s,\mathbf{k}) - i|\mathbf{k}>\frac{\hat{D}_{c(t-s)}(\mathbf{k})}{|\mathbf{k}|^2}\dot{\hat{\rho}}(s,\mathbf{k})]ds, \tag{12.18}$$

which through integration by parts becomes

$$\hat{C}(t,\mathbf{k}) = \hat{\mathcal{M}}_{ct}(\mathbf{k})\hat{C}_0(\mathbf{k}) - 4\pi c\int_0^t[\hat{\mathcal{M}}_{c(t-s)}(\mathbf{k})\hat{\mathbf{j}}(s,\mathbf{k}) - i|\mathbf{k}>\frac{\hat{D}'_{c(t-s)}(\mathbf{k})}{|\mathbf{k}|^2}\hat{\rho}(s,\mathbf{k})]ds. \tag{12.19}$$

Using $\hat{D}'_\tau(\mathbf{k}) = |\mathbf{k}| \sin |\mathbf{k}|\tau = |\mathbf{k}|^2 \hat{K}_\tau(\mathbf{k})$, we get

$$\mathcal{M}^{com}_\tau(\mathbf{x}) := F^{-1}\hat{\mathcal{M}}_\tau(\mathbf{k}) = K'_\tau(\mathbf{x}) - i\text{rot} \circ K_\tau(\mathbf{x}), \tag{12.20}$$

$$g^{com}_\tau(\mathbf{x}) := F^{-1}\Big(i|\mathbf{k} > \hat{K}_\tau(\mathbf{k}),\ -\hat{\mathcal{M}}_\tau(\mathbf{k})\Big) = (-\nabla K_\tau(\mathbf{x}),\ -\mathcal{M}^{com}_\tau(\mathbf{x})), \tag{12.21}$$

where $K_\tau(x)$ denotes the Kirchhoff kernel

$$K_\tau(\mathbf{x}) := F^{-1}\hat{K}_\tau(\mathbf{k}) = \frac{1}{4\pi\tau}\delta(|\mathbf{x}| - |\tau|). \tag{12.22}$$

With these notations, (12.19) implies then (12.4) in the "complex" form

$$C(t,\mathbf{x}) = \mathcal{M}^{com}_{ct} * C_0 + 4\pi \int_0^t g^{com}_{c(t-s)} * \begin{pmatrix} c\rho(s) \\ \mathbf{j}(s) \end{pmatrix} ds \quad t \in \mathbb{R}. \tag{12.23}$$

Separating into real and imaginary parts we obtain

$$E(t,\mathbf{x}) = E_{(r)}(t,\mathbf{x}) + E_{(0)}(t,\mathbf{x}), \quad B(t,\mathbf{x}) = B_{(r)}(t,\mathbf{x}) + B_{(0)}(t,\mathbf{x}), \tag{12.24}$$

$$\begin{pmatrix} E_{(0)}(t,\mathbf{x}) \\ B_{(0)}(t,\mathbf{x}) \end{pmatrix} = \mathcal{M}^{com}_{ct} * \begin{pmatrix} E_0 \\ B_0 \end{pmatrix} = \begin{pmatrix} K'_{ct} & \text{rot} \circ K_{ct} \\ -\text{rot} \circ K_{ct} & K'_{ct} \end{pmatrix} * \begin{pmatrix} E_0 \\ B_0 \end{pmatrix}, \tag{12.25}$$

$$\begin{pmatrix} E_{(r)}(t,\mathbf{x}) \\ B_{(r)}(t,\mathbf{x}) \end{pmatrix} = 4\pi \int_0^t \begin{pmatrix} -\nabla K_{c(t-s)} & -K'_{c(t-s)} \\ 0 & \text{rot} \circ K_{ct} \end{pmatrix} * \begin{pmatrix} c\rho(s) \\ \mathbf{j}(s) \end{pmatrix} ds. \tag{12.26}$$

13 Scattering and Long-Time Asymptotics

Let us discuss an outstanding role of the retarded potentials which are particular solutions of wave equations and Maxwell Eqns.

13.1 Retarded fields and local long-time asymptotics

The formula (12.26) may be rewritten as

$$E_{(r)}(t,\mathbf{x}) = -\nabla\phi_{(r)}(t,\mathbf{x}) - \frac{1}{c}\dot{A}_{(r)}(t,\mathbf{x}), \qquad B_{(r)}(t,\mathbf{x}) = \text{rot } A_{(r)}(t,\mathbf{x}), \tag{13.1}$$

where the potentials are given by

$$\phi_{(r)}(t,\mathbf{x}) = \int \frac{\Theta(t_{ret})}{|\mathbf{x}-\mathbf{y}|}\rho(t_{ret},\mathbf{y})d\mathbf{y}, \qquad A_{(r)}(t,\mathbf{x}) = \frac{1}{c}\int \frac{\Theta(t_{ret})}{|\mathbf{x}-\mathbf{y}|}\mathbf{j}(t_{ret},\mathbf{y})d\mathbf{y}, \tag{13.2}$$

where $t_{ret} = t - |\mathbf{x}-\mathbf{y}|/c$. Let us assume that the charge and current density are continuous and space-localized,

$$\rho(t,\mathbf{x}) = 0, \qquad \mathbf{j}(t,\mathbf{x}) = 0, \qquad |\mathbf{x}| > R, \ \ t \in \mathbb{R}. \tag{13.3}$$

Then (13.2) for large $t > 0$ become the standard *retarded potentials* [8],

$$\left\{ \begin{array}{lll} \phi_{(r)}(t,\mathbf{x}) & = \phi_{ret}(t,\mathbf{x}) & := \displaystyle\int \frac{\rho(t-|\mathbf{x}-\mathbf{y}|/c,\mathbf{y})}{|\mathbf{x}-\mathbf{y}|}d\mathbf{y} \\ A_{(r)}(t,\mathbf{x}) & = A_{ret}(t,\mathbf{x}) & := \displaystyle\frac{1}{c}\int \frac{\mathbf{j}(t-|\mathbf{x}-\mathbf{y}|/c,\mathbf{y})}{|\mathbf{x}-\mathbf{y}|}d\mathbf{y} \end{array} \right| \qquad t > R + |\mathbf{x}|. \tag{13.4}$$

Respectively, the fields (13.1) become the standard *retarded fields*

$$\left\{ \begin{array}{lll} E_{(r)}(t,\mathbf{x}) & = E_{(r)}(t,\mathbf{x}) & := -\nabla\phi_{ret}(t,\mathbf{x}) - \dot{A}_{ret}(t,\mathbf{x}), \\ B_{(r)}(t,\mathbf{x}) & = B_{(r)}(t,\mathbf{x}) & := \text{rot } A_{ret}(t,\mathbf{x}), \end{array} \right| \qquad t > R + |\mathbf{x}|. \tag{13.5}$$

An outstanding role of the particular retarded solutions (13.4) to the wave equations (11.6), (11.9) is justified in the *Scattering Theory*. Namely, the solutions to the wave equations (11.6), (11.9) are defined uniquely by the initial conditions at time zero:

$$\phi|_{t=0} = \phi_0(\mathbf{x}), \qquad \dot{\phi}|_{t=0} = \pi_0(\mathbf{x}), \qquad \mathbf{x} \in \mathbb{R}^3. \tag{13.6}$$

$$\mathcal{A}|_{t=0} = \mathcal{A}_0(\mathbf{x}), \qquad \dot{\mathcal{A}}|_{t=0} = \Pi_0(\mathbf{x}). \qquad \mathbf{x} \in \mathbb{R}^3. \tag{13.7}$$

However, the **asymptotic behavior** of the solutions for $t \to +\infty$ and any **fixed** point $\mathbf{x}$ does not depend on the initial data $\phi_0, \pi_0, \mathcal{A}_0, \Pi_0$ and coincide with the retarded potentials (13.4).

13.2 Space-localized initial data

For example let us consider the initial functions with compact supports.

Proposition 13.1 *Let (13.3) hold, and let the initial functions $\phi_0(x), \pi_0(x), \mathcal{A}_0(x), \Pi_0(x)$ be continuous and space-localized,*

$$\phi_0(\mathbf{x}) = \pi_0(\mathbf{x}) = 0, \qquad A_0(\mathbf{x}) = \Pi_0(\mathbf{x}) = 0, \qquad |\mathbf{x}| > R. \tag{13.8}$$

Then for large time the solutions to the Cauchy problems (11.6), (13.6) and (11.9), (13.7) coincide with the retarded potentials (13.4):

$$\phi(t,\mathbf{x}) = \phi_{ret}(t,\mathbf{x}), \qquad A(t,\mathbf{x}) = A_{ret}(t,\mathbf{x}), \qquad t > R + |\mathbf{x}|. \tag{13.9}$$

Proof Let us prove the proposition for the scalar potential $\phi(t,\mathbf{x})$. The Kirchhoff formula for the solution reads

$$\phi(t,\mathbf{x}) = \int_{S_t(\mathbf{x})} \pi_0(\mathbf{y}) dS(\mathbf{y}) + \partial_t \int_{S_t(\mathbf{x})} \phi_0(\mathbf{y}) dS(\mathbf{y}) + \phi_{ret}(t,\mathbf{x}), \qquad t > 0, \quad \mathbf{x} \in \mathbb{R}^3, \tag{13.10}$$

where $S_t(\mathbf{x})$ denotes the sphere $\{\mathbf{y} \in \mathbb{R}^3 : |\mathbf{x} - \mathbf{y}| = t\}$ and $dS(\mathbf{y})$ is the Lebesgue measure in the sphere. Now (13.9) follows from (13.8). ■

Similar theorem holds for the Maxwell Equations.

Theorem 13.2 *Let (13.3) and the conditions of the Theorem 12.1 hold, and*

$$E_0(\mathbf{x}) = B_0(\mathbf{x}) = 0, \qquad |\mathbf{x}| > R. \tag{13.11}$$

Then

$$E(t,\mathbf{x}) = E_{ret}(t,\mathbf{x}), \qquad B(t,\mathbf{x}) = B_{ret}(t,\mathbf{x}) \qquad t > R + |\mathbf{x}|. \tag{13.12}$$

Proof (13.12) follows from (12.24) and (13.5) since $E_{(0)}, B_{(0)}$ vanish for $t > R + |\mathbf{x}|$ by (13.11), (12.25) and (12.5). ■

13.3 Finite energy initial data

For the *free* Maxwell Eqns the energy is conserved, (12.3). For the wave equations (11.6) and (11.9) the energy conservations read (see (10.9)),

$$\int_{\mathbb{R}^3} [\frac{1}{c^2}|\dot\phi(t,\mathbf{x})|^2 + |\nabla\phi(t,\mathbf{x})|^2] d\mathbf{x} = \text{const}, \qquad \int_{\mathbb{R}^3} [\frac{1}{c^2}|\dot A(t,\mathbf{x})|^2 + |\nabla A(t,\mathbf{x})|^2] d\mathbf{x} = \text{const}. \tag{13.13}$$

For the finite energy initial solutions (13.9) and (13.12) hold in the local energy seminorms in the limit $t \to +\infty$.

Theorem 13.3 *Let (13.3) hold and $\phi(t,\mathbf{x})$ resp. $A(t,\mathbf{x})$ resp. $E(t,\mathbf{x}), B(t,\mathbf{x})$ are finite energy solutions to the wave equations (11.6) resp. (11.9) resp. the Maxwell Eqns (11.1). Then for any $R > 0$,*

$$\left\{ \begin{array}{l} \displaystyle\int_{|\mathbf{x}|<R} [|\ \dot\phi(t,\mathbf{x}) - \dot\phi_{ret}(t,\mathbf{x})|^2 + |\ \nabla\phi(t,\mathbf{x}) - \nabla\phi_{ret}(t,\mathbf{x})|^2] d\mathbf{x} \to 0 \\ \displaystyle\int_{|\mathbf{x}|<R} [|\dot A(t,\mathbf{x}) - \dot A_{ret}(t,\mathbf{x})|^2 + |\nabla A(t,\mathbf{x}) - \nabla A_{ret}(t,\mathbf{x})|^2] d\mathbf{x} \to 0 \\ \displaystyle\int_{|\mathbf{x}|<R} [|\dot E(t,\mathbf{x}) - \dot E_{ret}(t,\mathbf{x})|^2 + |\dot B(t,\mathbf{x}) - \dot B_{ret}(t,\mathbf{x})|^2] d\mathbf{x} \to 0 \end{array} \right| \quad t \to +\infty. \tag{13.14}$$

Proof Let us split the initial functions in two components: first, space-localized similar to (13.8),(13.11), and the rest. For the solutions corresponding to the localized components, the convergences (13.14) follow from (13.9) and (13.12). The contributions of the rest components are uniformly small in time by energy conservation. ■

14 Lagrangian theory for the Maxwell Field

14.1 4D vector potential

Let us introduce the four-dimensional notations

$$\left\{\begin{array}{ll} x_0 = ct, & x = (x_0, ..., x_3), \quad \partial_\mu = \nabla_\mu = (\partial_0, \partial_1, \partial_2, \partial_3), \\ g_{\mu\nu} = \mathrm{diag}(1, -1, -1, -, 1), & \partial^\mu := g_{\mu\nu}\partial_\nu = (\partial_0, -\partial_1, -\partial_2, -\partial_3). \end{array}\right. \tag{14.1}$$

Let us also introduce the 4D fields and currents

$$\left\{\begin{array}{ll} \mathcal{A}^\mu(x) = (\phi(t,\mathbf{x}), A(x)), & \mathcal{A}_\mu(x) := g_{\mu\nu}\mathcal{A}^\nu(x) = (\phi(x), -A(x)), \\ \mathcal{J}^\mu(x) = (\rho(x), \frac{1}{c}\mathbf{j}(x)), & \mathcal{J}_\mu(x) := g_{\mu\nu}\mathcal{J}^\nu(x) = (\rho(x), -\frac{1}{c}\mathbf{j}(x)). \end{array}\right. \quad x \in \mathbb{R}^4 \tag{14.2}$$

Then the Maxwell equations (11.6), (11.9) become

$$\Box\mathcal{A}^\mu(x) = 4\pi\mathcal{J}^\mu(x), \quad x \in \mathbb{R}^4. \tag{14.3}$$

Similarly, the charge continuity Eqn (11.2), gauge transformation (11.4) and the Lorentz gauge (11.5) become

$$\partial_\mu\mathcal{J}^\mu(x) = 0, \quad \mathcal{A}_\mu(x) \mapsto \mathcal{A}_\mu(x) + \partial^\mu\chi(x), \quad \partial_\mu\mathcal{A}^\mu(x) = 0, \quad x \in \mathbb{R}^4. \tag{14.4}$$

14.2 Tensor field

Definition 14.1 *The Maxwell tensor* $\mathcal{F}^{\mu\nu}(x) = \partial^\mu\mathcal{A}^\nu(x) - \partial^\nu\mathcal{A}^\mu(x)$, $x \in \mathbb{R}^4$.

Proposition 14.2 *The Maxwell Equations (14.3) are equivalent to*

$$\partial_\mu\mathcal{F}^{\mu\nu}(x) = 4\pi\mathcal{J}^\nu(x), \quad x \in \mathbb{R}^4. \tag{14.5}$$

Proof The Maxwell tensor does not depend on the choice of gauge since $\partial^\mu\partial^\nu\chi(x) - \partial^\nu\partial^\mu\chi(x) = 0$. Therefore, we can assume the Lorentz gauge (11.5) without loss of generality. Then (14.3) implies

$$\partial_\mu\mathcal{F}^{\mu\nu}(x) = \partial_\mu(\partial^\mu\mathcal{A}^\nu(x) - \partial^\nu\mathcal{A}^\mu(x)) = \partial_\mu\partial^\mu\mathcal{A}^\nu(x) = \Box\mathcal{A}^\nu(x) = 4\pi\mathcal{J}^\nu(x), \quad x \in \mathbb{R}^4. \tag{14.6}$$

■

14.3 Lagrangian density

Definition 14.3 *The Lagrangian density for the Maxwell Equations (14.5) with the* **given** *charge-current densities* $\mathcal{J}^\nu(x)$ *is defined by*

$$\mathcal{L}(x, \mathcal{A}_\mu, \nabla\mathcal{A}_\mu) = -\frac{1}{16\pi}\mathcal{F}^{\mu\nu}\mathcal{F}_{\mu\nu} - \mathcal{J}^\nu(x)\mathcal{A}_\nu, \quad (x, \mathcal{A}_\mu, \nabla\mathcal{A}_\mu) \in \mathbb{R}^4 \times \mathbb{R}^4 \times \mathbb{R}^{16}. \tag{14.7}$$

where $\mathcal{F}^{\mu\nu} := \partial^\mu\mathcal{A}^\nu - \partial^\nu\mathcal{A}^\mu$ *and* $\mathcal{F}_{\mu\nu} := \partial_\mu\mathcal{A}_\nu - \partial_\nu\mathcal{A}_\mu$.

Proposition 14.4 *The Maxwell Equations (14.5) with the given charge-current densities* $\mathcal{J}^\nu(x)$ *are equivalent to the Euler-Lagrange Eqns (6.10) with the Lagrangian density (14.7) for the fields* $\mathcal{A}_\mu(x)$.

Proof $\mathcal{F}_{\mu\nu}\mathcal{F}^{\mu\nu}$ is the quadratic form in $\nabla\mathcal{A}$. Therefore, the canonically conjugate fields π_α with the components $\pi_{\alpha\beta}$ are given by

$$\pi_{\alpha\beta} := \nabla_{\partial_\alpha\mathcal{A}_\beta}\mathcal{L} = -\frac{1}{8\pi}\mathcal{F}^{\mu\nu}\nabla_{\partial_\alpha\mathcal{A}_\beta}\mathcal{F}_{\mu\nu} = -\frac{1}{8\pi}(\mathcal{F}^{\alpha\beta} - \mathcal{F}^{\beta\alpha}) = -\frac{1}{4\pi}\mathcal{F}^{\alpha\beta}. \tag{14.8}$$

Therefore,

$$\nabla_\alpha\pi_{\alpha\beta}(x) = -\frac{1}{4\pi}\nabla_\alpha\mathcal{F}^{\alpha\beta}(x), \quad x \in \mathbb{R}^4. \tag{14.9}$$

On the other hand, $\partial_{\mathcal{A}_\beta}\mathcal{L} = -\mathcal{J}_\beta(x)$, hence (14.5) is equivalent to (6.10). ■

14.4 Lagrangian for charged particle in Maxwell Field

In a **continuous** Maxwell field the motion of the charged particle with small velocity $|\dot{\mathbf{q}}(t)| \ll c$ is governed by the Lorentz equation (L) from the Introduction,

$$m\ddot{\mathbf{q}}(t) = e[E(t,\mathbf{q}(t)) + \frac{1}{c}\dot{\mathbf{q}}(t) \times B(t,\mathbf{q}(t))], \quad t \in \mathbb{R}, \tag{14.10}$$

where m is the mass of the particle and e its charge. For large velocities $|\dot{\mathbf{q}}(t)| \sim c$ the equation must be replaced by

$$\dot{\mathbf{p}}(t) = e[E(t,\mathbf{q}(t)) + \frac{1}{c}\dot{\mathbf{q}}(t) \times B(t,\mathbf{q}(t))], \quad t \in \mathbb{R}, \tag{14.11}$$

where $\mathbf{p} := m\dot{\mathbf{q}}/\sqrt{1-(\dot{\mathbf{q}}/c)^2}$ is the relativistic momentum of the particle (see (5.6)). Let us assume that the fields E, B are C^1 vector-functions in $\mathbb{R}^4$. Then the dynamical equations (14.10), (14.11) define the corresponding dynamics uniquely. Let us define the charge-current densities $\mathcal{J}^\nu(t,\mathbf{x})$ corresponding to the trajectory $\mathbf{q}(\cdot)$: by (14.2),

$$\mathcal{J}^0(t,\mathbf{x}) = e\delta(x-\mathbf{q}(t)), \qquad \mathcal{J}^k(t,\mathbf{x}) = \frac{1}{c}\dot{\mathbf{q}}_k(t)e\delta(x-\mathbf{q}(t)), \quad k=1,2,3. \tag{14.12}$$

Let us show that the dynamical equations (14.10), (14.11) *follow automatically* from the Hamilton LAP applied to the Lagrangian density (14.7) with the fixed fields $E(t,\mathbf{x}), B(t,\mathbf{x})$. Namely, let us consider (14.10) for concreteness. Let $\mathcal{A}(t,\mathbf{x})$ be the 4-potential corresponding to the fields $E(t,\mathbf{x}), B(t,\mathbf{x})$. The Lagrangian density (14.7) consists of two parts: the field part $\mathcal{L}_f$ and the *field-matter interaction* part $\mathcal{L}_{fm}$. Substituting (14.12) into $\mathcal{L}_{fm}$, we get the field-matter action in the form

$$\begin{aligned} S^T_{fm}: &= \int_0^T \int_{\mathbb{R}^3} \mathcal{J}^\nu(t,\mathbf{x})\mathcal{A}_\nu(t,\mathbf{x})d\mathbf{x}\,dt \\ &= e\int_0^T \Big[\phi(t,\mathbf{q}(t)) - \frac{1}{c}\dot{\mathbf{q}}(t)\cdot A(t,\mathbf{q}(t))\Big]dt. \end{aligned} \tag{14.13}$$

The interaction term corresponds to the following Lagrangian function for the nonrelativistic particle,

$$L(\mathbf{q},\mathbf{v},t) = \frac{m\mathbf{v}^2}{2} - e\phi(t,\mathbf{q}) + \not{e}\mathbf{v}\cdot A(t,\mathbf{q}), \tag{14.14}$$

where $\not{e} := e/c$.

Theorem 14.5 *Let the potential $\mathcal{A}(t,\mathbf{x})$ be fixed. Then the Lorentz Equation (14.10) for the trajectory $\mathbf{q}(\cdot)$ is equivalent to the Euler-Lagrange equations corresponding to the Lagrangian (14.14)*

Proof First let us evaluate the momentum. By the definition, $\mathbf{p} := L_{\mathbf{v}} = m\mathbf{v} + \not{e}\,A(t,\mathbf{q})$, hence

$$\mathbf{p}(t) := L_{\mathbf{v}}(\mathbf{q}(t),\dot{\mathbf{q}}(t),t) = m\dot{\mathbf{q}}(t) + \not{e}\,A(t,\mathbf{q}(t)). \tag{14.15}$$

Now (3.15) becomes,

$$\dot{\mathbf{p}}_k(t) = L_{\mathbf{q}_k}(\mathbf{q}(t),\dot{\mathbf{q}}(t),t) = -e\nabla_k\phi(t,\mathbf{q}) + \not{e}\dot{\mathbf{q}}\cdot\nabla_k A(t,\mathbf{q})], \qquad k=1,2,3. \tag{14.16}$$

Let us calculate the derivative in the LHS:

$$\dot{\mathbf{p}}_k(t) = \frac{d}{dt}(m\dot{\mathbf{q}}_k(t) + \not{e}\, A_k(t, \mathbf{q}(t))) = m\ddot{\mathbf{q}}_k + \not{e}\,[\dot{A}_k(t, \mathbf{q}) + \nabla_j A_k(t, \mathbf{q})\dot{\mathbf{q}}_j]. \tag{14.17}$$

Substituting this expression into the LHS of (14.16), we get

$$m\ddot{\mathbf{q}}_k + \not{e}\,[\dot{A}_k(t, \mathbf{q}) + \nabla_j A_k(t, \mathbf{q})\dot{\mathbf{q}}_j] = -e\nabla_k\phi(t, \mathbf{q}) + \not{e}\dot{\mathbf{q}}_j\nabla_k A_j(t, \mathbf{q}). \tag{14.18}$$

Let us rewrite it as follows:

$$m\ddot{\mathbf{q}}_k = e[-\nabla_k\phi(t, \mathbf{q}) - \frac{1}{c}\,\dot{A}_k(t, \mathbf{q})] + \not{e}\,\dot{\mathbf{q}}_j[\nabla_k A_j - \nabla_j A_k]. \tag{14.19}$$

The first square bracket in the RHS is $E(t, \mathbf{x})$ by (11.3). Hence it remains to check that $\dot{\mathbf{q}}_j[\nabla_k A_j - \nabla_j A_k] = \dot{\mathbf{q}} \times \text{rot } A(t, \mathbf{x})$. Let us note that $\nabla_k A_j - \nabla_j A_k = (\text{rot } A)_l \varepsilon_{kjl}$ where ε_{kjl} is the antisymmetric tensor. Therefore, $\dot{\mathbf{q}}_j[\nabla_k A_j - \nabla_j A_k] = \dot{\mathbf{q}}_j(\text{rot } A)_l\varepsilon_{kjl} = [\dot{\mathbf{q}} \times \text{rot } A(t, \mathbf{x})]_k$ by definition of the vector product. ■

Remark 14.6 *The derivation of the expression for the Lorentz Force from the Maxwell Equations is not very surprising since the expression follows also from Coulomb and Biot-Savart-Laplace equation.*

14.5 Hamiltonian for charged particle in Maxwell Field

14.5.1 Nonrelativistic particle

We evaluate the Hamilton function as the Legendre transform of the nonrelativistic Lagrangian (14.14): first,

$$H := \mathbf{pv} - L = \mathbf{pv} - \frac{m\mathbf{v}^2}{2} + e\phi(t, \mathbf{q}) - \not{e}\mathbf{v} \cdot A(t, \mathbf{q}) = e\phi(t, \mathbf{q}) + \mathbf{v}(\mathbf{p} - \not{e}A(t, \mathbf{q})) - \frac{m\mathbf{v}^2}{2}. \tag{14.20}$$

Next we eliminate $\mathbf{v}$ by the relation $\mathbf{p} - \not{e}A(t, \mathbf{q}) = m\mathbf{v}$. Then we get finally,

$$H = e\phi(t, \mathbf{q}) + \frac{m\mathbf{v}^2}{2} = e\phi(t, \mathbf{q}) + \frac{1}{2m}(\mathbf{p} - \not{e}A(t, \mathbf{q}))^2. \tag{14.21}$$

14.5.2 Relativistic particle

Let us consider relativistic Lagrangian (cf. (5.6))

$$L(\mathbf{q}, \mathbf{v}, t) = -mc^2\sqrt{1 - \beta^2} - e\phi(t, \mathbf{q}) + \not{e}\mathbf{v} \cdot A(t, \mathbf{q}), \tag{14.22}$$

where $\beta := |\mathbf{v}|/c$. Let us note that the first term in the RHS is asymptotically $-mc^2 + m\mathbf{v}^2/2$ for $\beta \ll 1$. First we evaluate the momentum: by the definition, $\mathbf{p} := L_{\mathbf{v}} = m\mathbf{v}/\sqrt{1 - \beta^2} + \not{e}\, A(t, \mathbf{q})$, hence

$$\begin{aligned} H: &= \mathbf{pv} - L = \mathbf{pv} + mc^2\sqrt{1 - \beta^2} + e\phi(t, \mathbf{q}) - \not{e}\mathbf{v} \cdot A(t, \mathbf{q}) \\ &= e\phi(t, \mathbf{q}) + \mathbf{v}(\mathbf{p} - \not{e}A(t, \mathbf{q})) + mc^2\sqrt{1 - \beta^2}. \end{aligned} \tag{14.23}$$

Next we eliminate $\mathbf{p}$ by the relation $\mathbf{p} - \not{e}A(t, \mathbf{q}) = m\mathbf{v}/\sqrt{1 - \beta^2}$. Then we get,

$$\begin{aligned} H &= e\phi(t, \mathbf{q}) + \frac{m\mathbf{v}^2}{\sqrt{1 - \beta^2}} + mc^2\sqrt{1 - \beta^2} = e\phi(t, \mathbf{q}) + \frac{mc^2}{\sqrt{1 - \beta^2}} \\ &= e\phi(t, \mathbf{q}) + mc^2\sqrt{1 + (\mathbf{p} - \not{e}A(t, \mathbf{q}))^2/(mc)^2}\,. \end{aligned} \tag{14.24}$$

We can rewrite this relation in the following standard form

$$(H/c - \not{e}\phi(t,\mathbf{q}))^2 = m^2c^2 + (\mathbf{p} - \not{e}A(t,\mathbf{q}))^2 \,. \tag{14.25}$$

Remark 14.7 *This expression coincides with (1.1) for* $\phi = 0$, $A = 0$.

15 Maxwell Field in Matter

15.1 Missing matter equation

The Maxwell equations (11.1) define correctly the electromagnetic field generated by a given charge and current distribution. On the other hand, the Lorentz Equations (14.10), (14.11) define the motion of the charged particles in a given Maxwell field. However the classical theory cannot explain the structure of the matter i.e. the stability of particles, constitution of the atoms and molecules, solid state etc. This is related to the fact that the coupled system (11.1), (14.10) (or (11.1), (14.10)) is not well defined. Hence, we miss a correct dynamical equation for the matter.

15.2 Point charges

In 1897 J.J. Thomson suggested the existence of the electron as a point charged particle. Consider the coupled system (11.1), (14.10) for the point charge i.e. with charge and current densities (14.2). The coupled system is not well defined. Namely, the fields $\mathcal{A}^\nu(t,\mathbf{x})$ satisfy (11.1) hence they are singular functions at the points $\mathbf{x}=\mathbf{q}(t)$, $\mathcal{A}^\nu(t,\mathbf{x}) \sim |\mathbf{x}-\mathbf{q}(t)|^{-1}$. For example, the static solution to the stationary Poisson equation $-\Delta\phi(\mathbf{x}) = 4\pi\delta(x)$ is the Coulomb potential $\phi(\mathbf{x}) = |x|^{-1}$. Therefore, the RHS of the Lorentz Equations (14.10), (14.11) are not defined at the points $\mathbf{x}=\mathbf{q}(t)$. Thus, the dynamical description of the self-action for the point electron in the Classical Electrodynamics is impossible.

15.3 Abraham's extended electron

Abraham introduced the model of extended electron with a *rigid* charge shape $\rho(\mathbf{x}-\mathbf{q}(t))$ where the function $\rho(x)$ is fixed. Then the Lorentz Equation (14.10) is replaced by

$$m\ddot{\mathbf{q}}(t) = \int_{\mathbb{R}^3} [E(t,\mathbf{x}) + \frac{1}{c}\,\dot{\mathbf{q}}(t)\times B(t,\mathbf{x})]\rho(\mathbf{x}-\mathbf{q}(t))\,d\mathbf{x}, \quad t\in\mathbb{R}. \tag{15.1}$$

Now the coupled equations (15.1), (11.1) are well defined if we set $\rho(t,\mathbf{x}) := \rho(\mathbf{x}-\mathbf{q}(t))$ and $\mathbf{j}(t,\mathbf{x}) := \dot{\mathbf{q}}(t)\rho(\mathbf{x}-\mathbf{q}(t))$. However the problem arises on the right choice of the function $\rho(x)$. The Maxwell theory does not give any suggestion for the choice. So the dynamical description of the electron in Classical Electrodynamics requires additional hypothesis.

15.4 The Lorentz Theory of the molecular structure

Similarly, we have to introduce external hypothesis concerning the molecular structure, the charge and current distributions in the molecules etc., to describe the matter in the Maxwell field. Let us consider the matter as the collection of *identical small* cells called as *molecule* and let us analyze the Maxwell field generated by the charge and current distributions of a molecule at rest.

15.4.1 Dipole approximations

Let us denote by $a>0$ the size of the molecule and choose the origin 'in its center', i.e. assume that

$$\rho(t,\mathbf{y}) = 0,\ \ \mathbf{j}(t,\mathbf{y}) = 0, \quad |x|>a,\ \ t\in\mathbb{R}. \tag{15.2}$$

Let us assume that

$$\rho(t,\cdot) \in L^1(\mathbb{R}^3),\ \ \mathbf{j}(t,\cdot) \in L^1(\mathbb{R}^3) \otimes \mathbb{R}^3, \quad t \in \mathbb{R}. \tag{15.3}$$

Static fields First let us consider the static case when the densities do not depend on time. Then the equations (11.6), (11.9) become the stationary Poisson equations and its solution is the Coulombic potential

$$\phi(\mathbf{x}) = \int \frac{\rho(\mathbf{y})d\mathbf{y}}{|\mathbf{x}-\mathbf{y}|}, \qquad A(\mathbf{x}) = \frac{1}{c}\int \frac{\mathbf{j}(\mathbf{y})d\mathbf{y}}{|\mathbf{x}-\mathbf{y}|}, \qquad \mathbf{x} \in \mathbb{R}^3. \tag{15.4}$$

Let us expand the $1/|\mathbf{x}-\mathbf{y}|$ in the Taylor series for small $|\mathbf{y}| \le a$:

$$\frac{1}{|\mathbf{x}-\mathbf{y}|} = \frac{1}{\sqrt{\mathbf{x}^2+\mathbf{y}^2-2\mathbf{y}\mathbf{x}}} = \frac{1}{|\mathbf{x}|} + \frac{\mathbf{y}\mathbf{x}}{|\mathbf{x}|^3} + \mathcal{O}\left(\frac{1}{|\mathbf{x}|^3}\right), \qquad |\mathbf{x}| \to \infty. \tag{15.5}$$

Then (15.4) becomes,

$$\left\{ \begin{array}{l} \phi(\mathbf{x}) = \dfrac{Q}{|\mathbf{x}|} + \dfrac{\mathbf{p}\mathbf{x}}{|\mathbf{x}|^3} + \mathcal{O}\left(\dfrac{1}{|\mathbf{x}|^3}\right) \\ \\ A(\mathbf{x}) = \dfrac{J}{c|\mathbf{x}|} + \dfrac{\mathcal{M}\mathbf{x}}{|\mathbf{x}|^3} + \mathcal{O}\left(\dfrac{1}{|\mathbf{x}|^3}\right) \end{array} \right| \qquad |\mathbf{x}|/a \to \infty, \tag{15.6}$$

where we denote

$$\begin{array}{l} Q := \displaystyle\int \rho(\mathbf{y})d\mathbf{y}, \quad \mathbf{p} := \int \mathbf{y}\rho(\mathbf{y})d\mathbf{y}, \\ \\ J := \displaystyle\int \mathbf{j}(\mathbf{y})d\mathbf{y}, \quad \mathcal{M}_{kl} := \frac{1}{c}\int \mathbf{j}_k(\mathbf{y})\mathbf{y}_l d\mathbf{y}. \end{array} \tag{15.7}$$

We will identify the molecular fields with first two terms in the expansions (15.6) since $|\mathbf{x}|/a \gg 1$ in all *macro-observations*.

Let us note that the remainder in (15.5) is also $\mathcal{O}(\mathbf{y}^2)$. Therefore, first two terms in the expansions (15.6) correspond to the following *dipole approximations* for $\rho(\mathbf{y})$ and $\mathbf{j}(\mathbf{y})$:

$$\rho_d(\mathbf{y}) = Q\delta(\mathbf{y}) - \mathbf{p}\cdot\nabla_{\mathbf{y}}\delta(\mathbf{y}), \qquad \mathbf{j}_d(\mathbf{y}) = J\delta(\mathbf{y}) - c\mathcal{M}\nabla_{\mathbf{y}}\delta(\mathbf{y}). \tag{15.8}$$

Let us note that $Q = 0$ for the neutral molecule and then the main part of the molecular field is defined by the *dipole electric momentum* $\mathbf{p}$. For the *ions* the charge $Q \neq 0$.

Nonstationary fields It is easy to see that asymptotics of the type (15.6) hold for the *retarded* Kirchhoff potentials (13.4)) generated by nonstationary localized densities satisfying (15.2). Similarly to (15.8), we will identify the molecular charge and current densities with their dipole approximations

$$\rho_d(t,\mathbf{y}) = Q(t)\delta(\mathbf{y}) - \mathbf{p}(t)\cdot\nabla_{\mathbf{y}}\delta(\mathbf{y}), \qquad \mathbf{j}_d(t,\mathbf{y}) = J(t)\delta(\mathbf{y}) - c\mathcal{M}(t)\nabla_{\mathbf{y}}\delta(\mathbf{y}), \tag{15.9}$$

where $\mathcal{M}(t)$ is a real 3×3-matrix.

15.4.2 Multipole approximations

Let us note that it is possible to continue the Taylor expansion (15.5) and obtain a complete asymptotics of the type (15.6) including all negative powers of $|\mathbf{x}-\mathbf{y}|$. The asymptotics correspond to the following *multipole approximations* for $\rho(\mathbf{y})$ and $\mathbf{j}(\mathbf{y})$:

$$\text{(15.10)}\qquad \begin{cases} \rho_m(t,\mathbf{y}) = Q(t)\delta(\mathbf{y}) - \mathbf{p}(t)\cdot\nabla_{\mathbf{y}}\delta(\mathbf{y}) + \sum_{|\alpha|\geq 2}\rho_\alpha(t)\nabla^\alpha_{\mathbf{y}}\delta(\mathbf{y}), \\ \\ \mathbf{j}_m(t,\mathbf{y}) = J(t)\delta(\mathbf{y}) - c\mathcal{M}(t)\nabla_{\mathbf{y}}\delta(\mathbf{y}) + \sum_{|\alpha|\geq 2}\mathbf{j}_\alpha(t)\nabla^\alpha_{\mathbf{y}}\delta(\mathbf{y}). \end{cases}$$

The coefficients are defined by

$$\text{(15.11)}\qquad \begin{cases} \rho_\alpha(t) = \displaystyle\int_{\mathbb{R}^3}\frac{(-\mathbf{y})^\alpha}{\alpha!}\rho(t,\mathbf{y})d\mathbf{y} \\ \\ \mathbf{j}_\alpha(t) = \displaystyle\int_{\mathbb{R}^3}\frac{(-\mathbf{y})^\alpha}{\alpha!}\mathbf{j}(t,\mathbf{y})d\mathbf{y} \end{cases}$$

Let us justify the convergence of the series (15.10) in the sense of distributions.

Definition 15.1 *The space $\mathcal{H}_a(\mathbb{R}^3)$ consists of the test functions $\psi(\mathbf{y})$ which are real analytic in the ball $B_a = \{\mathbf{y}\in\mathbb{R}^3 : |\mathbf{y}| < a\}$ and the Taylor series $\psi(\mathbf{y}) = \sum_\alpha \frac{\mathbf{y}^\alpha}{\alpha!}\psi^{(\alpha)}(0)$ converge uniformly in B_a.*

Proposition 15.2 *Let (15.2) hold and $\rho(t,\cdot),\mathbf{j}(t,\cdot)\in L^1(\mathbb{R}^3)$. Then the series (15.10) converge and coincides with $\rho(t,\mathbf{y})$ resp. $\mathbf{j}(t,\mathbf{y})$ in the following sense:*

$$\text{(15.12)}\qquad \begin{cases} \langle\rho(t,\mathbf{y}),\psi(\mathbf{y})\rangle = \langle Q(t)\delta(\mathbf{y}) - \mathbf{p}(t)\cdot\nabla_{\mathbf{y}}\delta(\mathbf{y}) + \sum_{|\alpha|\geq 2}\rho_\alpha(t)\nabla^\alpha_{\mathbf{y}}\delta(\mathbf{y}),\psi(y)\rangle \\ \\ \langle\mathbf{j}(t,\mathbf{y}),\Psi(\mathbf{y})\rangle = \langle J(t)\delta(\mathbf{y}) - c\mathcal{M}(t)\nabla_{\mathbf{y}}\delta(\mathbf{y}) + \sum_{|\alpha|\geq 2}\mathbf{j}_\alpha(t)\nabla^\alpha_{\mathbf{y}}\delta(\mathbf{y}),\Psi(y)\rangle \end{cases}$$

for every test function from the space $\psi\in\mathcal{H}_a(\mathbb{R}^3)$ resp. $\Psi\in\mathcal{H}_a(\mathbb{R}^3)\otimes\mathbb{R}^3$.

Corollary 15.3 *The multipole approximations (15.10) satisfy the charge continuity equation*

$$\text{(15.13)}\qquad \dot\rho_m(t,\mathbf{y}) + \nabla_{\mathbf{y}}\cdot\mathbf{j}_m(t,\mathbf{y}) = 0, \qquad (t,\mathbf{y})\in\mathbb{R}^4.$$

Exercise 15.4 *Prove the corollary.* **Hint:** *Use the identity $\langle\dot\rho_m(t,\mathbf{y}) + \nabla_{\mathbf{y}}\cdot\mathbf{j}_m(t,\mathbf{y}),\psi(y)\rangle = \langle\dot\rho(t,\mathbf{y}) + \nabla_{\mathbf{y}}\cdot\mathbf{j}(t,\mathbf{y}),\psi(y)\rangle$ for $\psi\in\mathcal{H}_a(\mathbb{R}^3)$.*

Substituting the series (15.10) into (15.13), we get

$$\text{(15.14)}\qquad \dot Q(t)\delta(\mathbf{y}) - \dot{\mathbf{p}}(t)\cdot\nabla_{\mathbf{y}}\delta(\mathbf{y}) + J(t)\cdot\nabla_{\mathbf{y}}\delta(\mathbf{y}) + \sum_{|\alpha|\geq 2}C_\alpha(t)\nabla^\alpha_{\mathbf{y}}\delta(\mathbf{y}) = 0.$$

Therefore, we have

$$\text{(15.15)}\qquad \dot Q(t)\equiv 0, \qquad J(t)\equiv\dot{\mathbf{p}}(t).$$

Exercise 15.5 *Prove the Propositon 15.2.* **Hint:** *Substitute the Taylor expansion for ψ into the LHS of (15.12) and use (15.2).*

Exercise 15.6 *Check that the function* $\psi_{\mathbf{x}}(\mathbf{y}) := 1/|\mathbf{x}-\mathbf{y}|$ *belongs to the space* $\mathcal{H}_a(\mathbb{R}^3)$ *for any fixed* $\mathbf{x} \in \mathbb{R}^3 \setminus B_a$.

Now the static potentials (15.4) become the converging series

$$(15.16) \qquad \left\{ \begin{array}{l} \phi(\mathbf{x}) = \langle \rho(\mathbf{y}), \psi_{\mathbf{x}}(\mathbf{y}) \rangle = \dfrac{Q}{|\mathbf{x}|} + \dfrac{\mathbf{px}}{|\mathbf{x}|^3} + \displaystyle\sum_{|\alpha|\geq 2} \frac{\phi_\alpha}{|\mathbf{x}|^{|\alpha|+1}} \\ \\ A(\mathbf{x}) = \langle \mathbf{j}(\mathbf{y}), \psi_{\mathbf{x}}(\mathbf{y}) \rangle = \dfrac{J}{c|\mathbf{x}|} + \dfrac{\mathcal{M}\mathbf{x}}{|\mathbf{x}|^3} + \displaystyle\sum_{|\alpha|\geq 2} \frac{A_\alpha}{|\mathbf{x}|^{|\alpha|+1}} \end{array} \right| \qquad |\mathbf{x}| > a.$$

Exercise 15.7 *Check that the converging series also are asymptotic ones as* $|\mathbf{x}| \to \infty$.

Exercise 15.8 *Let (15.2) hold and the functions* $\rho(t,\mathbf{x})$, $\mathbf{j}(t,\mathbf{x})$ *be continuous. Prove the long-range asymptotics of type (15.16) for the retarded potentials (13.4)) and calculate first terms.*

15.4.3 Magnetic momentum of a molecule at stationary state

Let us consider a molecule in a stationary state, i.e. $\rho(t,\mathbf{y}) \equiv \rho(\mathbf{y})$ and $\mathbf{j}(t,\mathbf{y}) \equiv \mathbf{j}(\mathbf{y})$. Then also the multipole expansions (15.10) do not depend on time, i.e.

$$(15.17) \qquad \left\{ \begin{array}{l} \rho_m(t,\mathbf{y}) \equiv \rho_m(\mathbf{y}) = Q\delta(\mathbf{y}) - \mathbf{p}\cdot\nabla_{\mathbf{y}}\delta(\mathbf{y}) + \sum_{|\alpha|\geq 2} \rho_\alpha \nabla^\alpha_{\mathbf{y}}\delta(\mathbf{y}) \\ \\ \mathbf{j}_m(t,\mathbf{y}) \equiv \mathbf{j}_m(\mathbf{y}) = J\delta(\mathbf{y}) - c\mathcal{M}\nabla_{\mathbf{y}}\delta(\mathbf{y}) + \sum_{|\alpha|\geq 2} \mathbf{j}_\alpha \nabla^\alpha_{\mathbf{y}}\delta(\mathbf{y}). \end{array} \right.$$

Proposition 15.9 *Let the multipole charge-current densities (15.17) correspond to a stationary state of the molecule. Then the matrix* $\mathcal{M}$ *is skewsymmetric, and*

$$(15.18) \qquad \mathcal{M}\nabla_{\mathbf{y}} = \mathbf{m} \times \nabla_{\mathbf{y}},$$

where $\mathbf{m} \in \mathbb{R}^3$ *is the* **magnetic momentum** *of the molecule, i.e. of the current density* $\mathbf{j}(\mathbf{y})$, *in the stationary state.*

Proof Substituting (15.17) into (15.13), we get

$$(15.19) \qquad \nabla_{\mathbf{y}} \cdot \mathbf{j}_m(\mathbf{y}) = 0, \qquad \mathbf{y} \in \mathbb{R}^3.$$

Therefore in particular $\nabla_{\mathbf{y}} \cdot [\mathcal{M}\nabla_{\mathbf{y}}\delta(\mathbf{y})] = 0$. Then $\mathcal{M}_{kl} + \mathcal{M}_{lk} = 0$ and the vector $\mathbf{m} \in \mathbb{R}^3$ is defined by the following matrix identity:

$$(15.20) \qquad \mathcal{M} = \begin{pmatrix} 0 & -\mathbf{m}_3 & \mathbf{m}_2 \\ \mathbf{m}_3 & 0 & -\mathbf{m}_1 \\ -\mathbf{m}_2 & \mathbf{m}_1 & 0 \end{pmatrix} \qquad \blacksquare$$

The formulas (15.20) and (15.7) imply that

$$(15.21) \qquad \mathbf{m} = \frac{1}{2c} \int \mathbf{y} \times \mathbf{j}(\mathbf{y}) d\mathbf{y}.$$

Remark 15.10 *The integral does not depend on the choice of the origin if* $J := \int \mathbf{j}(\mathbf{y})d\mathbf{y} = 0$.

Adiabatic Condition Let us assume that the molecular dynamics can be described as an *adiabatic evolution* of the stationary states with corresponding magnetic momentum $\mathbf{m}(t)$.

Finally let us assume that the molecule is neutral, i.e. $Q = 0$, then (15.9) becomes by (15.15) and (15.18),

$$\rho_d(t,\mathbf{x}) = -\nabla_{\mathbf{x}} \cdot \mathbf{p}(t)\delta(\mathbf{x}), \qquad \mathbf{j}_d(t,\mathbf{x}) = \dot{\mathbf{p}}(t)\delta(\mathbf{x}) + c\nabla_{\mathbf{x}} \times \mathbf{m}(t)\delta(\mathbf{x}). \tag{15.22}$$

15.5 Maxwell Equations in Matter

15.5.1 Macroscopic Limit

The total molecular fields are generated by the sum of the charge-current densities $\rho_d^n(t,\mathbf{x})$, $\rho_d^n(t,\mathbf{x})$ of all molecules concentrated at the points $\mathbf{x}^n \in \mathbb{R}^3$:

$$\begin{cases} \rho_{\rm mol}(t,\mathbf{x}) & = \sum_n \rho_d^n(t,\mathbf{x}) & = -\sum_n \nabla_{\mathbf{x}} \cdot \mathbf{p}^n(t)\,\delta(\mathbf{x}-\mathbf{x}^n) \\ \mathbf{j}_{\rm mol}(t,\mathbf{x}) & = \sum_n \mathbf{j}_d^n(t,\mathbf{x}) & = \sum_n \left[\dot{\mathbf{p}}^n(t)\delta(\mathbf{x}-\mathbf{x}^n) + c\nabla_{\mathbf{x}} \times \mathbf{m}^n(t)\delta(\mathbf{x}-\mathbf{x}^n)\right] \end{cases} \tag{15.23}$$

Let us *assume* that for every fixed t we have the following asymptotics in the sense of distributions of $\mathbf{x}$:

$$\left.\begin{cases} \sum_n \mathbf{p}^n(t)\delta(\mathbf{x}-\mathbf{x}^n) \to P(t,\mathbf{x}) \\ \sum_n \dot{\mathbf{p}}^n(t)\delta(\mathbf{x}-\mathbf{x}^n) \to \dot{P}(t,\mathbf{x}), \qquad \sum_n \mathbf{m}^n(t)\delta(\mathbf{x}-\mathbf{x}^n) \to M(t,\mathbf{x}) \end{cases}\right| \; a \to 0. \tag{15.24}$$

Then by the continuity of the differentiation of the distributions, we have in the limit $a \to 0$,

$$\begin{cases} \rho_{\rm mol}(t,\mathbf{x}) & \approx -\nabla_{\mathbf{x}} \cdot P(t,\mathbf{x}) \\ \mathbf{j}_{\rm mol}(t,\mathbf{x}) & \approx \dot{P}(t,\mathbf{x}) + c\nabla_{\mathbf{x}} \times M(t,\mathbf{x}) \end{cases} \tag{15.25}$$

Definition 15.11 *The vector-function* $P(t,\mathbf{x})$ *resp.* $M(t,\mathbf{x})$ *is called the* **electric polarization** *resp.* **magnetization** *of the molecules at point* $\mathbf{x}$ *and time* t.

15.5.2 Dielectric Displacement and Magnetic field Intensity

Definition 15.12 $D(t,\mathbf{x}) = E(t,\mathbf{x}) + 4\pi P(t,\mathbf{x})$ *is called the dielectric displacement and* $H(t,\mathbf{x}) = B(t,\mathbf{x}) - 4\pi M(t,\mathbf{x})$ *is called the magnetic field intensity.*

Let us separate the macroscopic and molecular charge and current densities:

$$\rho(t,\mathbf{x}) = \rho_{\rm mac}(t,\mathbf{x}) + \rho_{\rm mol}(t,\mathbf{x}), \qquad \mathbf{j}(t,\mathbf{x}) = \mathbf{j}_{\rm mac}(t,\mathbf{x}) + \mathbf{j}_{\rm mol}(t,\mathbf{x}) \tag{15.26}$$

where the molecular densities are identified with the macroscopic limits (15.25). Let us substitute the expressions (15.26), (15.25) into the Maxwell Equations (11.1) and express the fields E, B in D, P, H, M. Then we obtain the *Maxwell Equations in the matter*:

$$\left.\begin{cases} \text{div } D(t,\mathbf{x}) = 4\pi\rho_{\rm mac}(t,\mathbf{x}), & \text{rot } E(t,\mathbf{x}) = -\dfrac{1}{c}\dot{B}(t,\mathbf{x}), \\ \text{div } B(t,\mathbf{x}) = 0, & \text{rot } H(t,\mathbf{x}) = \dfrac{1}{c}\dot{H}(t,\mathbf{x}) + \dfrac{4\pi}{c}\mathbf{j}_{\rm mac}(t,\mathbf{x}) \end{cases}\right| \; (t,\mathbf{x}) \in \mathbb{R}^4. \tag{15.27}$$

15.5.3 Constitutive Equations

The equations (15.27) contain two additional unknown vector fields D, H. Therefore, we need two additional vector equations. For **isotropic** materials there are the **constitutive equations**

$$D(t,\mathbf{x}) = \varepsilon E(t,\mathbf{x}), \qquad B(t,\mathbf{x}) = \mu H(t,\mathbf{x}), \tag{15.28}$$

where ε is called **the permittivity** and μ is called **the permeability** of the matter. The **constitutive equations** are equivalent to

$$P(t,\mathbf{x}) = \chi_e E(t,\mathbf{x}), \qquad M(t,\mathbf{x}) = \chi_m H(t,\mathbf{x}), \tag{15.29}$$

where χ_e is called **the electric susceptibility** and χ_m is called **the magnetic susceptibility** of the matter. The following relations follow from Definition 15.12:

$$\varepsilon = 1 + 4\pi\chi_e, \qquad \mu = 1 + 4\chi_m. \tag{15.30}$$

16 Schrödinger Eqn and Geometric Optics

Wave equations of type (11.12) describe the wave propagation in electrodynamics, acoustics and many other fields. They describe well the diffraction and the interference of waves. On the other hand, the wave processes also demonstrate the straight-line propagation of waves which justifies Geometric Optics. The mathematical description of this feature by the wave equation has been discovered by Hamilton around 1830 and developed by Liouville in 1837, Debye in 1911, Rayleigh in 1912, Jeffreys in 1923, and Schrödinger, Wentzel, Kramers and Brillouin in 1926.

16.1 Straightline Propagation for the Free Equations

Let us analyze the straight-line propagation in the concrete example of the **free** Klein-Gordon Equation

$$\left\{ \begin{array}{l} \ddot\psi(t,\mathbf{x}) = \Delta\psi(t,\mathbf{x}) - m^2\psi(t,\mathbf{x}) \\ \psi(0,\mathbf{x}) = \psi_0(\mathbf{x}),\ \ \dot\psi(0,\mathbf{x}) = \pi_0(\mathbf{x}) \end{array} \right| \qquad (t,\mathbf{x}) \in \mathbb{R}\times\mathbb{R}^3. \tag{16.1}$$

Let us choose the initial data $\psi_0(\mathbf{x}), \pi_0(\mathbf{x})$ from the *Schwartz space* $\mathcal{S}(\mathbb{R}^3)$ of test functions.

Definition 16.1 *$\mathcal{S}(\mathbb{R}^3)$ is the space of functions $\psi(\mathbf{x}) \in C^\infty(\mathbb{R}^3)$ such that*

$$\sup_{\mathbf{x}\in\mathbb{R}^3} (1+|\mathbf{x}|)^N |\nabla^\alpha_{\mathbf{x}}\psi(\mathbf{x})| < \infty \tag{16.2}$$

for any $N = 1, 2, ...$ and multiindices $\alpha = (\alpha_1, \alpha_2, \alpha_3)$.

Definition 16.2 *For $\psi \in \mathcal{S}(\mathbb{R}^3)$ the Fourier transform is defined by*

$$F\psi(\mathbf{k}) := \hat\psi(\mathbf{k}) := (2\pi)^{-3}\int_{\mathbb{R}^3} e^{i\mathbf{k}\mathbf{x}}\psi(\mathbf{x})d\mathbf{x}, \quad \mathbf{k}\in\mathbb{R}^3. \tag{16.3}$$

Proposition 16.3 *Let $\psi_0, \pi_0 \in \mathcal{S}(\mathbb{R}^3)$. Then the Cauchy problem (16.1) admits a unique solution $\psi(t,\mathbf{x})$ satisfying the bounds*

$$\sup_{\mathbf{x}\in\mathbb{R}^3} (1+|\mathbf{x}|)^N |\nabla_t^{\alpha_0}\nabla^\alpha_{\mathbf{x}}\psi(t,\mathbf{x})| < C(\alpha_0,\alpha,N)(1+|t|)^N, \quad t\in\mathbb{R} \tag{16.4}$$

for any $N = 1, 2, ...$, $\alpha_0 = 0, 1, 2, ...$ and multiindices $\alpha = (\alpha_1, \alpha_2, \alpha_3)$.

Proof Let us calculate the solution to (16.1) with $\psi_0, \pi_0 \in \mathcal{S}(\mathbb{R}^3)$ by using the Fourier transform. Let us apply the transform to the equations (16.1) using well-known formulas

$$(F\partial_1\psi)(t,\mathbf{k}) = -ik_1\hat\psi(t,\mathbf{k}), \qquad (F\Delta\psi)(t,\mathbf{k}) = -k^2\hat\psi(t,\mathbf{k}), \qquad (t,\mathbf{k})\in\mathbb{R}\times\mathbb{R}^3. \tag{16.5}$$

The bounds (16.4) imply also that $(F\dot\psi)(t,\mathbf{k}) = \dot{\hat\psi}(t,\mathbf{k})$ and $(F\ddot\psi)(t,\mathbf{k}) = \ddot{\hat\psi}(t,\mathbf{k})$ hence (16.1) becomes

$$\left\{ \begin{array}{l} \ddot{\hat\psi}(t,\mathbf{k}) = -k^2\hat\psi(t,\mathbf{k}) - m^2\hat\psi(t,\mathbf{k}) \\ \hat\psi(0,\mathbf{k}) = \hat\psi_0(\mathbf{k}),\ \ \dot{\hat\psi}(0,\mathbf{k}) = \hat\pi_0(\mathbf{k}) \end{array} \right| \qquad (t,\mathbf{k})\in\mathbb{R}\times\mathbb{R}^3. \tag{16.6}$$

This is the Cauchy problem for the ordinary differential equation which depends on the parameter $\mathbf{k}\in\mathbb{R}^3$. The solution is well known,

$$\hat\psi(t,\mathbf{k}) = \hat\psi_0(\mathbf{k})\cos\omega t + \hat\pi_0(\mathbf{k})\frac{\sin\omega t}{\omega}, \qquad \omega = \omega(k) := \sqrt{k^2+m^2}. \tag{16.7}$$

Therefore, the solution $\psi(t,\mathbf{x})$ is given by the inverse Fourier transform,

$$\begin{aligned}\psi(t,\mathbf{x}) &= \int_{\mathbb{R}^3} e^{-i\mathbf{x}\mathbf{k}}\Big[\hat\psi_0(\mathbf{k})\cos\omega t + \hat\pi_0(\mathbf{k})\frac{\sin\omega t}{\omega}\Big]d\mathbf{x}\\ &= \frac{1}{2}\int_{\mathbb{R}^3} e^{-i\mathbf{x}\mathbf{k}}\Big[e^{i\omega t}\Big(\hat\psi_0(\mathbf{k})+\frac{\hat\pi_0(\mathbf{k})}{i\omega}\Big)+e^{-i\omega t}\Big(\hat\psi_0(\mathbf{k})-\frac{\hat\pi_0(\mathbf{k})}{i\omega}\Big)\Big]d\mathbf{k}\\ &= \psi_+(t,\mathbf{x})+\psi_-(t,\mathbf{x}). \qquad (16.8)\end{aligned}$$

The representation obviously implies the bounds (16.4) since $\hat\psi_0, \hat\pi_0 \in \mathcal{S}(\mathbb{R}^3)$. ■

Now let us choose the initial functions ψ_0, π_0 with a localized spectrum, i.e.

$$\text{supp}\ \hat\psi_0,\ \text{supp}\ \hat\pi_0 \subset B_r(\mathbf{k}_*), \qquad (16.9)$$

where $B_r(\mathbf{k}_*)$ is an *open* ball with a center $\mathbf{k}_* \in \mathbb{R}^3$ and a small radius $r \ll |\mathbf{k}_*|$. Then the same is true for the spectra of the functions $\psi_\pm(t,\mathbf{x})$ by (16.8):

$$\text{supp}\ \hat\psi_\pm(t,\cdot) \subset B_r(\mathbf{k}_*), \qquad t \in \mathbb{R}. \qquad (16.10)$$

The solutions of type $\psi_\pm(t,\mathbf{x})$ are called *wave packets*.

Theorem 16.4 *Let $\psi_0, \pi_0 \in \mathcal{S}(\mathbb{R}^3)$ and (16.9) holds. Then the corresponding wave packets $\psi_\pm(t,\mathbf{x})$ are localized solutions moving with the* **group velocities** $\mathbf{v}_\pm = \pm\nabla\omega(\mathbf{k}_*)$ *in the following sense:*
i) For a constant $a > 0$ and any $N > 0$,

$$|\psi_\pm(t,\mathbf{x})| \le C_N(1+|t|+|\mathbf{x}|)^{-N}, \quad |\mathbf{x}-\mathbf{v}_\pm t| > \frac{ar}{|\mathbf{k}_*|}|t|. \qquad (16.11)$$

ii) For any constant $A > 0$,

$$|\psi_\pm(t,\mathbf{x})| \le C(1+|t|)^{-3/2}, \qquad |\mathbf{x}-\mathbf{v}_\pm t| \le \frac{Ar}{|\mathbf{k}_*|}|t|. \qquad (16.12)$$

Proof Let us prove the theorem for ψ_+ since for ψ_- just the same arguments hold. Let us consider the function $\psi_+(t,\mathbf{x})$ along a ray $\mathbf{x} = \mathbf{v}t$ with an arbitrary $\mathbf{v} \in \mathbb{R}^3$: by (16.8),

$$\psi_+(t,\mathbf{v}t) = \int e^{-i\phi_+(\mathbf{k})t}\Psi_+(\mathbf{k})d\mathbf{k}. \qquad (16.13)$$

Here the *phase function* is given by $\phi_+(\mathbf{k}) := \mathbf{v}\mathbf{k} - \omega(\mathbf{k})$ and the amplitude $\Psi_+(\mathbf{k}) := \hat\psi_0(\mathbf{k})/2 + \hat\pi_0(\mathbf{k})/(2i\omega(\mathbf{k}))$. Let us apply the *method of the stationary phase* [6] to the integral (16.13). Then we get that the asymptotics for $t \to \infty$ depend on the existence of the critical points $\mathbf{k} \in \text{supp}\ \Psi_+$ of the phase function $\phi_+(\mathbf{k})$,

$$\nabla\phi_+(\mathbf{k}) = \mathbf{v} \mp \nabla\omega(\mathbf{k}) = 0, \quad \mathbf{k} \in \text{supp}\ \Psi_+. \qquad (16.14)$$

In other words, $\mathbf{v} = \nabla\omega(\mathbf{k})$ with a $\mathbf{k} \in \text{supp}\ \Psi_+$. Now let us take into account that $\text{supp}\ \Psi_+ \subset B_r(\mathbf{k}_*)$ by (16.9). Then the system (16.14) admits a solution iff $\mathbf{v} \in \mathbf{V}_r(\mathbf{k}_*) := \{\nabla\omega(\mathbf{k}) : \mathbf{k} \in B_r(\mathbf{k}_*)\}$. Now let us analyze two distinct situations separately.

i) First let us consider $\mathbf{v} \notin \mathbf{V}_r(\mathbf{k}_*)$. Then the asymptotics of the integral (16.13) is $|t|^{-N}$ for any

$N > 0$ which corresponds to (16.11). Let us deduce the asymptotics by a partial integration in (16.13) with the help of an obvious identity

$$e^{-i\phi_+(\mathbf{k})t} = \frac{D}{-it} e^{-i\phi_+(\mathbf{k})t}, \qquad \mathbf{k} \in \text{supp } \Psi_+, \tag{16.15}$$

where D is the following differential operator, $D = (\nabla\overline{\phi}(\mathbf{k})/|\nabla\phi(\mathbf{k})|^2) \cdot \nabla$. It is important that $\nabla\phi(\mathbf{k}) \neq 0$ for $\mathbf{k} \in \text{supp } \Psi_+$ since $\mathbf{v} \notin \mathbf{V}_r(\mathbf{k}_*)$. Applying N times the identity (16.15) in (16.13), we get by partial integration,

$$\psi_+(t, \mathbf{v}t) = (-it)^{-N} \int D^N e^{-i\phi_+(\mathbf{k})t} \Psi_+(\mathbf{k}) d\mathbf{k} = (-it)^{-N} \int e^{-i\phi_+(\mathbf{k})t} (D^*)^N \Psi_+(\mathbf{k}) d\mathbf{k}, \tag{16.16}$$

where $D^*\Psi(\mathbf{k}) = \nabla \cdot [\nabla\overline{\phi}(\mathbf{k})\Psi(\mathbf{k})/|\nabla\phi(\mathbf{k})|^2]$ is the adjoint operator to D. Therefore,

$$\psi_+(t, \mathbf{v}t) \leq C_N(\mathbf{v})(1 + |t|)^{-N}, \quad t \in \mathbb{R} \tag{16.17}$$

if $\mathbf{v} \notin \mathbf{V}_r(\mathbf{k}_*)$. Hence, for any $B > 0$,

$$\psi_+(t, \mathbf{v}t) \leq C_N(B)(1 + |t| + |\mathbf{v}t|)^{-N}, \quad t \in \mathbb{R} \tag{16.18}$$

if $\mathbf{v} \notin \mathbf{V}_r(\mathbf{k}_*)$ and $|\mathbf{v}| \leq B$.

Exercise 16.5 *Prove that the bounds (16.18) hold for all $\mathbf{v} \notin \mathbf{V}_r(\mathbf{k}_*)$ with a uniform constant C_N instead of $C_N(B)$.*
Hint: *Consider the function $\psi_+(t, \mathbf{x})$ along the ray $t = w\tau, x = v\tau$ with $|w| < 1$, $|v| = 1$ and apply the same partial integration with the phase function $\mathbf{k}v - w\omega(\mathbf{k})$ and large parameter $\tau \to \infty$.*

Finally, the bounds (16.18) with C_N instead of $C_N(B)$ imply (16.11) since the diameter of the set $\mathbf{V}_r(\mathbf{k}_*)$ does not exceed $ar/|\mathbf{k}_*|$. The last follows from the bound $|\nabla\nabla\omega(\mathbf{k})| \leq a/|\mathbf{k}|$ which is obvious since

$$\nabla\omega(\mathbf{k}) = \frac{\mathbf{k}}{\omega(\mathbf{k})}. \tag{16.19}$$

ii) It remains to consider $\mathbf{v} \in \mathbf{V}_r(\mathbf{k}_*)$. This means that $\mathbf{v} = \nabla\omega(\mathbf{k})$ with a point $\mathbf{k} \in B_r(\mathbf{k}_*)$ which is the solution to the system (16.14). Then the integral (16.13) is called the *Fresnel* integral and its asymptotics is $\sim |t|^{-3/2}$ (see [6]). ■

Remark 16.6 *The asymptotics (16.11), (16.12) mean that the energy of the field $\psi_\pm(t, \mathbf{x})$* **outside** *a ball $|\mathbf{x} - \mathbf{v}_\pm t| \leq ar|t|/|\mathbf{k}_*|$ decays rapidly, while* **inside** *it is about constant since the energy is a* **quadratic form**. *Therefore, the wave packet $\psi_\pm(t, \mathbf{x})$ of the* **free** *Klein-Gordon Equation (16.1) move like free particle of increasing size $\sim r|t|/|\mathbf{k}_*|$ and with the* **group velocity** $\mathbf{v}_\pm = \pm\nabla\omega(\mathbf{k}_*)$. *The formula (16.19) means that the velocity $\mathbf{v}_\pm$ corresponds to the relativistic momentum $\pm\mathbf{k}_*$ of the particle.*

Exercise 16.7 *Analyze the wave-packets propagation for the* **free** *Schrodinger equation*

$$\left\{ \begin{array}{rcl} -i\dot{\psi}(t, \mathbf{x}) & = & \dfrac{1}{2m} \Delta\psi(t, \mathbf{x}) \\ \\ \psi(0, \mathbf{x}) & = & \psi_0(\mathbf{x}), \end{array} \right| \qquad (t, \mathbf{x}) \in \mathbb{R} \times \mathbb{R}^3. \tag{16.20}$$

Prove that the packets move like **free** *nonrelativistic particles of increasing size $\sim r|t|/|\mathbf{k}_*|$ with the mass m and momentum $\mathbf{k}_*$.*
Hint: *$\omega = \mathbf{k}^2/2m$ hence the* **group velocity** $\mathbf{v}$ *equals $\nabla\omega = \mathbf{k}/m$.*

16.2 WKB-method for Schrödinger Eqn with a Maxwell Field

Let us write the Lorentz Eqn (14.10) in the Hamilton form with the Hamiltonian (14.21):

$$\left\{\begin{array}{rcl} \dot{\mathbf{q}} & = & H_{\mathbf{p}}(\mathbf{q},\mathbf{p},t) = \dfrac{1}{m}(p - \not{e}A(t,\mathbf{q})), \\ \dot{\mathbf{p}} & = & -H_{\mathbf{q}}(\mathbf{q},\mathbf{p},t) = -e\phi_{\mathbf{q}}(t,\mathbf{q}) + \dfrac{1}{m}\not{e}A_{\mathbf{q}}(t,\mathbf{q}), \end{array}\right. \tag{16.21}$$

where $\not{e} := e/c$, e is the charge of the particle and m its mass. E.Schrödinger associated with the Hamilton system the wave equation (S) (see Introduction):

$$(i\hbar\partial_t - e\phi(t,\mathbf{x}))\psi(t,\mathbf{x}) = \frac{1}{2m}(-i\hbar\nabla_{\mathbf{x}} - \not{e}A(t,\mathbf{x}))^2\psi(t,\mathbf{x}), \qquad (t,\mathbf{x}) \in \mathbb{R}^4. \tag{16.22}$$

Let us demonstrate that the short-wave solutions to (16.22) are governed by the Hamilton Eqns (16.21). More precisely, let us consider the Cauchy problem for (16.22) with the initial condition

$$\psi|_{t=0} = a_0(\mathbf{x})e^{iS_0(\mathbf{x})/\hbar}\ , \qquad \mathbf{x} \in \mathbb{R}^3, \tag{16.23}$$

where $S_0(\mathbf{x})$ is a real function. Let us denote by $(\mathbf{q}(t,\mathbf{q}_0),\mathbf{p}(t,\mathbf{q}_0))$ the solution to the Hamilton Eqns (16.21) with the initial conditions (5.8):

$$\mathbf{q}|_{t=0} = \mathbf{q}_0, \qquad \mathbf{p}|_{t=0} = \nabla S_0(\mathbf{q}_0). \tag{16.24}$$

The solution exists for $|t| < T(\mathbf{q}_0)$ where $T(\mathbf{q}_0) > 0$.

Definition 16.8 *The curve $x = \mathbf{q}(t,\mathbf{q}_0)$ is the* **Ray** *of the Cauchy problem (16.22), (16.23) starting at the point q_0.*

Definition 16.9 *The* **Ray Tube** *or* **Ray Beam emanating from the initial function** *(16.23) is the set $\mathcal{T} = \{(t,\mathbf{q}(t,\mathbf{q}_0)) \in \mathbb{R}^4 : |t| < T(\mathbf{q}_0), \quad \mathbf{q}_0 \in \text{supp } a_0\}$.*

The following theorem means roughly speaking that for $\hbar \ll 1$ the set $\mathcal{T}$ is the support of the wave function $\psi(t,\mathbf{x})$, the solution to the Cauchy problem (16.22), (16.23). Let us assume that the potentials $\phi(t,\mathbf{x}), A(t,\mathbf{x}) \in C^\infty(\mathbb{R}^4)$ and $a_0, S_0 \in C^\infty(\mathbb{R}^3)$. Then the map $\mathbf{q}_0 \mapsto \mathbf{q}(t,\mathbf{q}_0)$ is a local C^∞-diffeomorphism of $\mathbb{R}^3$ for small $|t|$. We will construct the formal *Debye expansion*

$$\psi(t,\mathbf{x}) \sim \Big(\sum_{k=0}^{\infty}\hbar^k a_k(t,\mathbf{x})\Big)e^{iS(t,\mathbf{x})/\hbar}\ , \qquad \hbar \to 0. \tag{16.25}$$

Theorem 16.10 *Let the map $\mathbf{q}_0 \mapsto \mathbf{q}(t,\mathbf{q}_0)$ be a diffeomorphism of $\mathbb{R}^3$ for $|t| < T$. Then the formal expansion (16.25) exists for $|t| < T$ and is identically zero outside $\mathcal{T}$, i.e.*

$$a_k(t,\mathbf{x}) = 0, \qquad (t,\mathbf{x}) \notin \mathcal{T}, \quad |t| < T, \quad k = 0,1,2,... \tag{16.26}$$

Proof First let us define the phase function $S(t,\mathbf{x})$ as the solution to the Cauchy problem (5.7) with $N = 3$:

$$\left\{\begin{array}{rcl} -\dot{S}(t,\mathbf{x}) & = & H(\mathbf{x},\nabla S(t,\mathbf{x}),t), \quad \mathbf{x} \in \mathbb{R}^3, \quad |t| < T, \\ S|_{t=0} & = & S_0(\mathbf{x}), \quad \mathbf{x} \in \mathbb{R}^3. \end{array}\right. \tag{16.27}$$

The solution exists by Theorem 5.10. Further, let us substitute $\psi(t,\mathbf{x}) = a(t,\mathbf{x})e^{iS(t,\mathbf{x})/\hbar}$ into the Schrödinger equation (16.22). Then the equation (16.27) implies the following *Transport Equation* for the amplitude $a(t,\mathbf{x})$:

$$
\left\{\begin{array}{rcl}
\dot a(t,\mathbf{x}) &=& -\dfrac{1}{m}[\nabla S(t,\mathbf{x}) - \not{A}(t,\mathbf{x})]\cdot\nabla a(t,\mathbf{x}) \\
&& +\dfrac{1}{2m}[\Delta S(t,\mathbf{x}) + \nabla\cdot A(t,\mathbf{x})]a(t,\mathbf{x}) + \dfrac{i\hbar}{2m}\Delta a(t,\mathbf{x}) \\
&=:& -La(t,\mathbf{x}) + B(t,\mathbf{x})a(t,\mathbf{x}) + \dfrac{i\hbar}{2m}d(t,\mathbf{x}), \quad |t|<T, \\
\\
a|_{t=0} &=& a_0(\mathbf{x}), \quad \mathbf{x}\in\mathbb{R}^3,
\end{array}\right. \tag{16.28}
$$

where L is the first order differential operator $La(t,\mathbf{x}) := \dfrac{1}{m}[\nabla S(t,\mathbf{x}) - \not{A}(t,\mathbf{x})]\cdot\nabla a(t,\mathbf{x})$, $B(t,\mathbf{x})$ is the function $\dfrac{1}{2m}[\Delta S(t,\mathbf{x}) + \nabla\cdot A(t,\mathbf{x})]$ and $d(t,\mathbf{x}) := \Delta a(t,\mathbf{x})$. Let us note that (16.21) implies

$$
\dot a(t,\mathbf{x}) + La(t,\mathbf{x}) = \frac{d}{dt}a(t,\mathbf{q}(t,\mathbf{q}_0)). \tag{16.29}
$$

Let us express all the functions in the *Ray Coordinates* $(t,\mathbf{q}_0)$: $\tilde a(t,\mathbf{q}_0) := a(t,\mathbf{q}(t,\mathbf{q}_0))$, $\tilde B(t,\mathbf{q}_0) := B(t,\mathbf{q}(t,\mathbf{q}_0))$ etc. Then (16.28) can be rewritten as

$$
\left\{\begin{array}{rcl}
\dfrac{d}{dt}\tilde a(t,\mathbf{q}_0) &=& \tilde B(t,\mathbf{q}_0)\tilde a(t,\mathbf{q}_0) + \dfrac{i\hbar}{2m}\tilde d(t,\mathbf{q}_0), \quad |t|<T, \\
\\
\tilde a(0,\mathbf{q}_0) &=& a_0(\mathbf{q}_0), \quad \mathbf{q}_0\in\mathbb{R}^3.
\end{array}\right. \tag{16.30}
$$

Let us substitute in the first equation the formal expansion $\tilde a(t,\mathbf{q}_0) \sim \sum\limits_{k=0}^{\infty}\hbar^k\tilde a_k(t,\mathbf{q}_0)$. Equating formally the terms with identical powers of $\hbar$, we get the recursive *Transport Equations*

$$
\left.\begin{array}{l}
\dfrac{d}{dt}\tilde a_0(t,\mathbf{q}_0) = \tilde B(t,\mathbf{q}_0)\tilde a_0(t,\mathbf{q}_0), \\
\\
\dfrac{d}{dt}\tilde a_1(t,\mathbf{q}_0) = \tilde B(t,\mathbf{q}_0)\tilde a_1(t,\mathbf{q}_0) + \dfrac{i}{2m}\tilde d_0(t,\mathbf{q}_0), \\
\\
\ldots \\
\\
\dfrac{d}{dt}\tilde a_k(t,\mathbf{q}_0) = \tilde B(t,\mathbf{q}_0)\tilde a_k(t,\mathbf{q}_0) + \dfrac{i}{2m}\tilde d_{k-1}(t,\mathbf{q}_0), \\
\\
\ldots
\end{array}\right| \quad |t|<T, \tag{16.31}
$$

where $\tilde d_0(t,\mathbf{q}_0)$ is the function $d_0(t,x) := \Delta a_0(t,x)$ expressed in the ray coordinates, etc. It remains to substitute the same expansion into the initial conditions (16.30) which gives

$$
\tilde a_0(0,\mathbf{q}_0) = a_0(\mathbf{q}_0), \quad \tilde a_1(0,\mathbf{q}_0) = 0, \quad \ldots, \quad \tilde a_k(0,\mathbf{q}_0) = 0, \ldots \tag{16.32}
$$

Now (16.31) and (16.32) imply that $\tilde a_0(t,\mathbf{q}_0) = 0$, $|t|<T$, if $\mathbf{q}_0 \notin \operatorname{supp} a_0$. Hence, also $\tilde d_0(t,\mathbf{q}_0) = 0$, $|t|<T$, if $\mathbf{q}_0 \notin \operatorname{supp} a_0$. Therefore, (16.31) and (16.32) imply that $\tilde a_1(t,\mathbf{q}_0) = 0$, $|t|<T$, if $\mathbf{q}_0 \notin \operatorname{supp} a_0$, etc. ■

Exercise 16.11 *Prove the transport equation (16.28).* **Hint:** *Substitute* $\psi = ae^{iS/\hbar}$ *into the Schrödinger Equation (16.22) and devide by* $e^{iS/\hbar}$*. Then the equation (16.27) formally follows by setting* $\hbar = 0$*, and afterwards, (16.28) also follows.*

17 Schrödinger Equation

17.1 Schrödinger Equation for the Electron Field

The *Electron* has been discovered by J.J.Thomson round 1897 in the *Cathode Rays*. He systematized the observations of the deflection of the rays in the Maxwell Field. The observations demonstrated that the deflection corresponds to the Newton dynamics (14.10) or (16.21) with a fixed ratio e/μ close to its present value. Later Kauffmann [10] confirmed the observations with a high accuracy $e/\mu \approx -1.76 \cdot 10^8 \mathrm{C/g}$. The charge of the electron can be evaluated from the Faraday Electrolyze Law $e \approx -96500\mathrm{C}/6.06 \cdot 10^{23} \approx 1.6 \cdot 10{-}19\mathrm{C} \approx -4.77 \cdot 10^{-10}$ esu. In 1913 Millikan confirmed the result $e \approx 1.60 \cdot 10^{-19}\mathrm{C} \approx -4.77 \cdot 10^{-10}$ esu, then the electron mass $\mu \approx 9.1 \cdot 10^{-28}\mathrm{g}$. Therefore, by Theorem 16.10, the cathode rays can be also described by the Schrödinger Eqn (16.22) with the mass $\mu > 0$ and *negative* value $e < 0$.

Remarks 17.1 *i) Let us note that the coefficients e, m are determined from the experiments with the cathode rays of an arbitrary charge. Therefore, the experiments fix the ratio e/m and do not fix the charge e. Hence, the corresponding Schrödinger Eqn (16.22) describe rather the dynamics of the Electron Field than the dynamics of a particle with the charge e.*
ii) Theorem 16.10 means that the Schrödinger Equation (16.22) with any small $\hbar \ll 1$ agrees with the classical Newton Eqns (14.10) or (16.21). The actual value of the constant is fixed by the Planck relation $\hbar = a/k \approx 1.05 \cdot 10^{-27} erg \cdot sec$. Here a is the parameter in the Wien experimental formula (W) (see Introduction) and k is the Boltzmann constant. This identification of the constant $\hbar$ in the Schrödinger Equation follows from the development of the quantum mechanics given by Planck, Einstein, Bohr, de Broglie and Schrödinger (see Introduction).

17.2 Static Maxwell Field

Let us consider the case of *static* Maxwell Field with the potentials $\phi(t, \mathbf{x}) \equiv \phi(\mathbf{x})$ and $A(t, \mathbf{x}) \equiv A(\mathbf{x})$:

$$i\hbar \partial_t \psi(t, \mathbf{x}) = H\psi(t, \cdot) := \frac{1}{2\mu}(-i\hbar \nabla_{\mathbf{x}} - \not{e}A(\mathbf{x}))^2 \psi(t, \mathbf{x}) + e\phi(\mathbf{x})\psi(t, \mathbf{x}), \qquad (t, \mathbf{x}) \in \mathbb{R}^4. \tag{17.1}$$

Then the energy is conserved (see (10.17)):

$$E(t) := \int_{\mathbb{R}^3} \Big[\frac{1}{2\mu}|(-i\hbar \nabla_{\mathbf{x}} - \not{e}A(\mathbf{x}))\psi(t, \mathbf{x})|^2 + e\phi(\mathbf{x})|\psi(t, \mathbf{x})|^2\Big] d\mathbf{x} = E, \qquad t \in \mathbb{R}. \tag{17.2}$$

Definition 17.2 Quantum Stationary States *for the Eqn (17.1) are nonzero finite energy solutions of type*

$$\psi(t, \mathbf{x}) = \psi_\omega(\mathbf{x}) e^{-i\omega t}. \tag{17.3}$$

Substituting (17.3) into (17.1), we get the *Stationary Schrödinger Eqn*

$$\hbar\omega \psi_\omega(\mathbf{x}) = H\psi_\omega(\mathbf{x}), \qquad \mathbf{x} \in \mathbb{R}^3, \tag{17.4}$$

which is the *eigenvalue problem*. Substituting (17.3) into (17.2) and using (17.4), we get the energy in the form

$$E = E_\omega = \hbar\omega \int_{\mathbb{R}^3} |\psi_\omega(\mathbf{x})|^2 d\mathbf{x}. \tag{17.5}$$

Let us assume the standard **Normalization**

$$\int_{\mathbb{R}^3} |\psi_\omega(\mathbf{x})|^2 d\mathbf{x} = 1. \tag{17.6}$$

Then (17.5) becomes (cf. (P) from Introduction)

$$E_\omega = \hbar\omega, \tag{17.7}$$

and (17.4) takes the form

$$E_\omega\psi_\omega(\mathbf{x}) = H\psi_\omega(\mathbf{x}), \qquad \mathbf{x}\in\mathbb{R}^3, \tag{17.8}$$

Remark 17.3 *The energy (17.2) can be represented as*

$$E(t)= \langle\psi(t,\cdot), H\psi(t,\cdot)\rangle, \tag{17.9}$$

where $\langle\cdot,\cdot\rangle$ stands for the scalar product in $L^2(\mathbb{R}^3)$.

17.3 Hydrogen Atom

Let us consider the Hydrogen Atom. This is the atom with a unique electron of the negative charge e. Rutherford experiment shows that the positive charge $-e$ is concentrated in very small region called "nucleus", so its Maxwell field is Coulombic $\phi(t,\mathbf{x}) = -e/|\mathbf{x}|$. We assume the magnetic field of the nucleus be zero: $A(t,\mathbf{x}) = 0$. Then the Schrödinger Eqn (17.1) becomes

$$i\hbar\partial_t\psi(t,\mathbf{x}) = H\psi(t,\mathbf{x}) := -\frac{\hbar^2}{2\mu}\Delta\psi(t,\mathbf{x}) - \frac{e^2}{|\mathbf{x}|}\psi(t,\mathbf{x}), \qquad (t,\mathbf{x})\in\mathbb{R}^4. \tag{17.10}$$

Respectively, the stationary Schrödinger Eqn (17.8) becomes,

$$E_\omega\psi_\omega(\mathbf{x}) = H\psi(\mathbf{x}) = -\frac{\hbar^2}{2\mu}\Delta\psi_\omega(\mathbf{x}) - \frac{e^2}{|\mathbf{x}|}\psi_\omega(\mathbf{x}), \qquad \mathbf{x}\in\mathbb{R}^3. \tag{17.11}$$

Theorem 17.4 *The quantum stationary states ψ_ω of the Hydrogen Atom exist for the energies $E_\omega = E_n := -R/n^2$, where $R := \mu e^4/(2\hbar^2)$ is the* **Ridberg Constant** *and $n = 1, 2, 3, \ldots$. For other energies the states do not exist.*

We will prove the theorem in next two Sections.

17.4 Spectral Theorem for Spherical Laplacian

Let us express the Laplacian operator Δ in the spherical coordinates r, ϕ, θ. By the definition

$$x_3 = r\cos\theta, \;\; x_1 = r\sin\theta\cos\varphi, \;\; x_2 = r\sin\theta\sin\varphi. \tag{17.12}$$

The operator Δ is symmetric in the real Hilbert space $L^2(\mathbb{R}^3)$. Hence it is defined uniquely by the quadratic form $(\Delta\psi,\psi)$, where $\psi\in D := \{\psi\in L^2(\mathbb{R}^3) : \psi^{(\alpha)}\in L^2(\mathbb{R}^3)\cap C(\mathbb{R}^3), \;\; |\alpha|\le 2\}$. In the spherical coordinates

$$(\Delta\psi,\psi) = -(\nabla\psi,\nabla\psi) = -\int_0^\infty dr\int_0^\pi d\theta\int_0^{2\pi} d\varphi|\nabla\psi(r,\theta,\varphi)|^2 r^2\sin\theta. \tag{17.13}$$

Geometrically is evident that

$$\nabla\psi(r,\theta,\varphi) = e_r\nabla_r\psi + e_\theta\frac{\nabla_\theta\psi}{r} + e_\varphi\frac{\nabla_\varphi\psi}{r\sin\theta}, \tag{17.14}$$

where e_r, e_θ, e_φ are the orthogonal unit vectors proportional to ∇_r, ∇_θ, ∇_φ, respectively. Therefore, (17.13) becomes

$$(17.15) \qquad (\Delta\psi,\psi) = -\int_0^\infty dr \int_0^\pi d\theta \int_0^{2\pi} d\varphi \Big(\Big|\nabla_r\psi\Big|^2 + \Big|\frac{\nabla_\theta\psi}{r}\Big|^2 + \Big|\frac{\nabla_\varphi\psi}{r\sin\theta}\Big|^2 \Big) r^2\sin\theta.$$

Integrating by parts, we get

$$\begin{aligned} (\Delta\psi,\psi) &= \int_0^\infty dr \int_0^\pi d\theta \int_0^{2\pi} d\varphi (r^{-2}\nabla_r r^2 \nabla_r\psi + \frac{\nabla_\theta \sin\theta \nabla_\theta\psi}{r^2\sin\theta} + \frac{\nabla_\varphi^2\psi}{r^2\sin^2\theta})\psi r^2\sin\theta \\ &= (r^{-2}\nabla_r r^2\nabla_r\psi + \frac{\nabla_\theta\sin\theta\nabla_\theta\psi}{r^2\sin\theta} + \frac{\nabla_\varphi^2\psi}{r^2\sin^2\theta}, \psi). \qquad (17.16) \end{aligned}$$

Therefore, we get the Laplacian operator in the spherical coordinates,

$$(17.17) \qquad \Delta\psi = r^{-2}\nabla_r r^2\nabla_r\psi + \frac{\nabla_\theta\sin\theta\nabla_\theta\psi}{r^2\sin\theta} + \frac{\nabla_\varphi^2\psi}{r^2\sin^2\theta} = r^{-2}\nabla_r r^2\nabla_r\psi + \frac{\Lambda}{r^2}\psi \ ,$$

where Λ is the differential operator on the sphere S with the coordinates θ,φ:

$$(17.18) \qquad \Lambda = \frac{\nabla_\theta\sin\theta\nabla_\theta\psi}{\sin\theta} + \frac{\nabla_\varphi^2\psi}{\sin^2\theta} \ ,$$

Definition 17.5 *Λ is the* **Spherical Laplacian operator**.

Exercise 17.6 *Check the integration by parts (17.16).*

Let dS denote the Lebesgue measure on the sphere S. Then the norm of the Hilbert space $L^2(S,dS)$ is invariant with respect to rotations.

Theorem 17.7 *There exist a representation $L^2(S,dS) = \oplus_{l=0}^\infty D(l)$ where $D(l) \subset C^\infty(S)$ are the orthogonal subspaces of $L^2(S,dS)$ of the odd dimension $2l+1$, and $\Lambda|_{D(l)} = -l(l+1)$.*

We will prove the theorem in next two Lectures. Here we apply it to the eigenvalue problem (17.11).

17.5 Spectrum of Hydrogen Atom

Here we deduce Theorem 17.4 from Theorem 17.7. Let us consider a nonzero finite energy solution $\psi_\omega(\mathbf{x}) \in L^2(\mathbb{R}^3)$ to the problem (17.11). We will prove that $E_\omega = E_n := -R/n^2$. First, expand

$$(17.19) \qquad \psi_\omega(\mathbf{x}) = \sum_0^\infty R_l(r)Y_l(\theta,\varphi),$$

where $Y_l(\theta,\varphi) \in D(l)$. The expansion exists and converges in $L^2(\mathbb{R}^3)$ by Theorem 17.7. Then the series converge also in the sense of distributions of $r>0, (\theta,\varphi) \in S$, hence

$$\begin{aligned} E_\omega\psi_\omega(\mathbf{x}) &= H\psi_\omega(\mathbf{x}) = \sum_0^\infty H(R_l(r)Y_l)(\theta,\varphi) \\ &= \sum_0^\infty \Big(-\frac{\hbar^2}{2\mu}[r^{-2}\nabla_r r^2\nabla_r R_l(r) - \frac{l(l+1)}{r^2}R_l(r)] - \frac{e^2}{r}R_l(r)\Big) Y_l(\theta,\varphi), \qquad (17.20) \end{aligned}$$

where the series also converge in the sense of the distributions. The orthogonality of Y_l implies for each $l = 0, 1, 2, ...,$

$$-\frac{2\mu E_\omega}{\hbar^2}R_l(r) = r^{-2}\nabla_r r^2 \nabla_r R_l(r) - \frac{l(l+1)}{r^2}R_l(r) + \frac{2\mu e^2}{\hbar^2 r}R_l(r), \quad r > 0. \tag{17.21}$$

For $r \to \infty$ the equation becomes

$$-\frac{2\mu E_\omega}{\hbar^2}R_l(r) \sim R_l''(r). \tag{17.22}$$

This suggests that $E_\omega < 0$ and the asymptotics holds $R_l(r) \sim e^{-\gamma r}$, $r \to \infty$, where

$$\gamma = \sqrt{-2\mu E}/\hbar > 0. \tag{17.23}$$

Respectively, let us write $R_l(r) = e^{-\gamma r}F(r)$. Substituting into (17.21), we get

$$F'' + \Big[\frac{2}{r} - 2\gamma\Big]F' + \Big[\frac{d}{r} - \frac{l(l+1)}{r^2}\Big]F = 0, \quad r > 0, \tag{17.24}$$

where $d = b - 2\gamma$ with $b = 2\mu e^2/\hbar^2$. Finally let us introduce new variable $\rho = 2\gamma r$, then (17.24) becomes

$$f'' + \Big[\frac{2}{\rho} - 1\Big]f' + \Big[\frac{\lambda - 1}{\rho} - \frac{l(l+1)}{\rho^2}\Big]f = 0, \quad \rho > 0, \tag{17.25}$$

where $f(\rho) = F(r)$ and $\lambda = b/(2\gamma)$. Now let us seak the solution f in the form

$$f(\rho) = \rho^s(a_0 + a_1\rho + a_2\rho^2 + ...) \equiv L(\rho)\rho^s \tag{17.26}$$

with $a_0 \neq 0$. We will find two linearly independent solutions: one with $s \geq 0$ and another with $s \leq -1$. Only the solution with $s \geq 0$ is appropriate. For $s \leq -1$ corresponding eigenfunction $\psi_\omega(x)$ is not the function of finite energy since $\nabla\psi_\omega(x) \notin L^2(\mathbb{R}^3)$ and $\int \phi(\mathbf{x})|\psi(\mathbf{x})|^2 d\mathbf{x} = \infty$. Substituting (17.26) into (17.25), we get

$$L''\rho^2 + \left[2s\rho + \Big[\frac{2}{\rho} - 1\Big]\rho^2\right]L' + \left[s(s-1) + \Big[\frac{2}{\rho} - 1\Big]s\rho + \Big[\frac{\lambda - 1}{r} - \frac{l(l+1)}{\rho^2}\Big]\rho^2\right]L = 0 \tag{17.27}$$

for $\rho > 0$. After some evaluation, we have

$$\rho^2 L'' + \rho[2(s+1) - \rho]L' + [\rho(\lambda - 1 - s) + s(s+1) - l(l+1)]L = 0, \quad \rho > 0. \tag{17.28}$$

Setting $\rho = 0$, we get formally $s(s+1) - l(l+1) = 0$. Hence, $s = l$ since $-l - 1 \leq -1$. With $s = l$, the equation becomes

$$\rho L'' + [2(s+1) - \rho]L' + [\lambda - 1 - s]L = 0, \quad \rho > 0. \tag{17.29}$$

Let us substitute here $L(\rho) = a_0 + a_1\rho + a_2\rho^2 + ...$ and equate the coefficients with identical powers of ρ:

$$\begin{cases} \rho^0: & 2(l+1) + (\lambda - 1 - l)a_0 = 0, \\ \rho^1: & 2a_2 + 2(l+1)2a_2 - a_1 + (\lambda - 1 - l)a_1 = 0, \\ \rho^2: & 3 \cdot 2a_3 + 2(l+1)3a_3 - 2a_2 + (\lambda - 1 - l)a_2 = 0, \\ & ... \\ \rho^k: & (k+1)ka_{k+1} + 2(l+1)(k+1)a_{k+1} - ka_k + (\lambda - 1 - l)a_k = 0, \\ & ... \end{cases} \tag{17.30}$$

Therefore, we get the recursive relation

$$a_{k+1} = \frac{k-(\lambda-1-l)}{(k+1)(k+2l+2)}a_k. \tag{17.31}$$

It implies $a_{k+1}/a_k \sim 1/k$ if all $a_k \neq 0$. Then we have $|L(\rho)| \geq Ce^{\rho} = Ce^{2\gamma r}$ with a $C > 0$. Hence, $R_l(r) = F(r)e^{-\gamma r} \to \infty$ as $r \to \infty$, which is impossible. Therefore, $a_{k+1} = 0$ and $a_k \neq 0$ for some $k = 0, 1, 2, ...$ Then $k - (\lambda - 1 - l) = 0$, so

$$\lambda = \frac{b}{2\gamma} = k + l + 1 = n = 1, 2, ... \tag{17.32}$$

Substituting here $b = 2\mu e^2/\hbar^2$ and $\gamma = \sqrt{-2\mu E}/\hbar$, we get finally,

$$E = E_n := -\frac{R}{n^2}, \qquad n = 1, 2, ..., \tag{17.33}$$

where $R := \mu e^4/(2\hbar^2)$. ■

Let us note that $L(\rho) = \rho^l(a_0 + ... + a_k\rho^k)$ is a polynomial of the degree $k + l = n - 1$. The value of $n - 1$ equals the number of the zeros of the function $L(\rho)$, $\rho \geq 0$, and n is called the **principal quantum number**.

Corollary 17.8 *The eigenfunctions ψ_ω for $\omega = E_n = -R/n^2$ have the following form in the spherical coordinates:*

$$\psi_\omega = Ce^{-\gamma r}P_{ln}(r)F_{lm}(\theta)e^{im\varphi}. \tag{17.34}$$

Here $\gamma = \gamma(\omega) > 0$, $P_{ln}(r)$ is a polynomial of the degree $n - 1 \geq l$, $F_{lm}(\theta)e^{im} \in D(l)$ and $m = -l, ..., l$.

Exercise 17.9 *Deduce (17.21) from (17.20).*

Exercise 17.10 *Calculate the multiplicity of the eigenvalue E_n.*
Hint: it is equal to the $\sum_{0\leq l\leq n-1}(2l+1)$.

18 Spherical Functions and Lie Algebras

Here we prove Theorem 17.7.

18.1 Spherical Symmetry and Angular Momentum Conservation

The basic idea in solving the eigenvalue problem (17.11) is its spherical symmetry which is equivalent to

$$[H, \nabla_\varphi] = 0, \tag{18.1}$$

where φ is the angle of rotation of the space $\mathbb{R}^3$ around an arbitrary unit vector $e \in \mathbb{R}^3$. The commutation holds by (17.11) since the Laplacian Δ and the Coulombic potential are invariant under all rotations of the space $\mathbb{R}^3$. Namely, the rotation invariance and (17.11) imply

$$HR_e(\varphi) - R_e(\varphi)H = 0, \qquad \varphi \in \mathbb{R}, \tag{18.2}$$

where $(R_e(\varphi)\psi)(\mathbf{x}) = \psi(O_e(\varphi)x)$ (see (9.11)). Differentiating (18.2) in φ at $\varphi = 0$ we get (18.1) since $\nabla_\varphi := \left.\dfrac{d}{d\varphi}\right|_{\varphi=0} R_e(\varphi)$.

Let us show that the commutation implies the conservation of the projection $M_e(t) = M(t)\cdot e$ of the angular momentum defined by (8.2). Let us fix an arbitrary unit vector $e \in \mathbb{R}^3$ and choose the coordinates in $\mathbb{R}^3$ in such a way that $e = e_3 := (0,0,1)$. Then according to the first equation in (10.21),

$$M_e(t) = \frac{i\hbar}{2}\int_{\mathbb{R}^3} \psi(t,\mathbf{x})\cdot(\mathbf{x}\times\nabla_{\mathbf{x}})_3\psi(t,\mathbf{x})d\mathbf{x} = \frac{i\hbar}{2}\int_{\mathbb{R}^3} \psi(t,\mathbf{x})\cdot\nabla_\varphi\psi(t,\mathbf{x})d\mathbf{x}. \tag{18.3}$$

Let us introduce the differential operator $M_e := \dfrac{i\hbar}{2}\nabla_\varphi$ and the Euclidean resp. Hermitian scalar product $(\cdot,\cdot)$ resp. $\langle\cdot,\cdot\rangle$ in the real resp. complex Hilbert space $L^2(\mathbb{R}^3)$:

$$(\psi_1(\mathbf{x}),\psi_2(\mathbf{x})) := \int_{\mathbb{R}^3}\psi_1(\mathbf{x})\cdot\psi_2(\mathbf{x})d\mathbf{x}, \qquad \langle\psi_1(\mathbf{x}),\psi_2(\mathbf{x})\rangle := \int_{\mathbb{R}^3}\psi_1(\mathbf{x})\overline{\psi_2(\mathbf{x})}d\mathbf{x}. \tag{18.4}$$

Then (18.3) becomes

$$M_e(t) = (\psi(t), M_e\psi(t)) = \langle\psi(t), M_e\psi(t)\rangle, \tag{18.5}$$

where $\psi(t) := \psi(t,\cdot)$.

Theorem 18.1 *For the solutions to the Schrödinger equation (17.10) the angular momentum M_e is conserved,*

$$M_e(t) = \text{const}. \tag{18.6}$$

Proof I The Lagrangian density (6.7) for the equation (17.1) satisfies the invariance condition (8.1). Hence, (18.6) holds by Theorem 8.3. ■

Proof II The conservation (18.6) follows directly from the commutation of the operators H and $M_e \sim \nabla_\varphi$: (18.1) implies

$$[H, M_e] = 0. \tag{18.7}$$

Therefore, differentiation of (18.5) gives by (17.10),

$$\begin{aligned} \dot{M}_e(t) &= \langle\dot{\psi}(t), M_e\psi(t)\rangle + \langle\psi(t), M_e\dot{\psi}(t)\rangle \\ &= \langle -iH\psi(t), M_e\psi(t)\rangle + \langle\psi(t), M_e(-iH\psi(t))\rangle \\ &= \langle\psi(t), i[HM_e - M_eH]\psi(t)\rangle = 0 \end{aligned} \tag{18.8}$$

since H is the *symmetric* operator in $L^2(\mathbb{R}^3)$. ■

Exercise 18.2 *Check that H is the symmetric operator in $L^2(\mathbb{R}^3)$.*

Further we identify the operators ∇_φ and M_e with the differential operators on S. Then the commutation (18.7) implies that

$$[\Lambda, \nabla_\varphi] = [\Lambda, M_e] = 0, \qquad e \in \mathbb{R}^3. \tag{18.9}$$

18.2 Spectral Theorem for Spherical Laplacian

Lemma 18.3 *The Spherical Laplacian Λ is an elliptic second order operator, positive definite and symmetric in $L^2(S, dS)$.*

Proof The ellipticity follows from (17.18). Λ is positive definite and symmetric in $L^2(S, dS)$ since Δ is positive definite and symmetric in $L^2(\mathbb{R}^3)$. ■
This lemma and the Elliptic Theory [13] imply the Spectral Resolution

$$L^2(S, dS) = \oplus_{j=0}^{\infty} L(j), \tag{18.10}$$

where $L(j) \subset C^\infty(S)$ are finite dimensional orthogonal subspaces of $L^2(S, dS)$ and $\Lambda|_{L(j)} = \lambda_j$ with $\lambda_j \neq \lambda_i$ for $j \neq i$. It remains to prove that $\dim L(j) = 2l + 1$ and $\lambda_j = 2l + 1$ with an $l = 0, 1, 2, \ldots$.

Lemma 18.4 *All spaces $L(j)$ are invariant with respect to the rotations of the sphere.*

Proof The invariance follows from the invariance of Λ.

Corollary 18.5 *For each unit vector $e \in \mathbb{R}^3$, all spaces $L(j)$ are invariant with respect to the operator $H_e := -i\nabla_\varphi$, where φ is the angle of the rotation around e.*

18.3 Lie Algebra of Angular Momenta

Let us denote by H_k, $k = 1, 2, 3$, the operators H_{e_k} corresponding to the vectors $e_1 = (1, 0, 0)$ etc. Then the linear span (H_1, H_2, H_3) is a Lie Algebra since

$$[H_1, H_2] = iH_3, \qquad [H_2, H_3] = iH_1, \qquad [H_3, H_1] = iH_2. \tag{18.11}$$

Exercise 18.6 *Check the commutators.* **Hint:** *$H_k = -i(\mathbf{x} \times \nabla_{\mathbf{x}})_k$, as in (18.3).*

Lemma 18.7 *For each $k = 1, 2, 3$,*
i) The operators H_k are symmetric in $L^2(S, dS)$.
ii) All spaces $L(j)$ are invariant with respect to H_k.
iii) $[\Lambda, H_k] = 0$.

Proof *ad i)* H_k are symmetric since the rotations around e_k are the unitary operators in $L^2(S, dS)$.
ad ii) The invariance holds by Corollary 18.5.
ad iii) The commutation holds by (18.9). ■

Definition 18.8 $H_\pm = H_1 \pm iH_2$.

Lemma 18.9 *i) All spaces $L(j)$ are invariant with respect to $H_\pm$.*
ii) $[\Lambda, H_\pm] = 0$.
iii) $[H_3, H_\pm] = \pm H_\pm$.

Proof *i*), *ii*) follow from Lemma 18.7, *iii*) follows from (18.11). ■

Let us fix an arbitrary j. Theorem 17.7 follows from

Theorem 18.10 *There exists an $l = 0, 1, 2, ...$ such that:*
i) There exists a basis $\{e_m : m = -l, ..., l\}$ in the space $L(j)$.
ii) $H_3 e_m = m e_m$.
iii) $\lambda_j = -l(l+1)$.

Proof H_3 is a symmetric operator in $L(j)$, hence H_3 admits a diagonal form in a basis of its eigenfunctions v_s in $L(j)$:

$$H_3 v_s(\theta, \varphi) = -i\nabla_\varphi v_s(\theta, \varphi) = s v_s(\theta, \varphi). \tag{18.12}$$

Therefore, $v_s(\theta, \varphi) = F(\theta) e^{is\varphi}$, so $s = m$ is an integer number.

Lemma 18.11 *Let m be an eigenvalue of H_3 in $L(j)$: $H_3 v_m(\theta, \varphi) = m v_m(\theta, \varphi)$ where $v_m \in L(j)$, $v \neq 0$. Then*
i) $-m$ also is an eigenvalue of H_3 in $L(j)$.
ii) Either $w_\pm := H_\pm v_m = 0$, or $w_\pm$ is an eigenfunction of H_3 in $L(j)$ with the eigenvalue $m \pm 1$.

Proof *ad i)* The function $v_m(\theta, -\varphi)$ is the solution to (18.12) with $s = -m$. It belongs to the same space $L(j)$ since the operator Λ is invariant under the symmetry $\varphi \mapsto -\varphi$ by (17.18).
ad ii) By Lemma 18.9 *iii*) we have $H_3 w = H_3 H_\pm v_m = H_\pm H_3 v_m \pm H_\pm v_m = m w_\pm \pm w_\pm$. ■

Corollary 18.12 *The set of all eigenvalues of the operator H_3 in $L(j)$ has the form $-l, ..., l$ where $l = 0, 1, 2, ...$*

It remains to prove that each eigenvalue is simple and $\lambda_j = -l(l+1)$.

First consider the lowest eigenvalue $m = -l$. Then $H_- v_{-l}(\theta, \varphi) = 0$ by Lemma 18.11. We will prove below that in the spherical coordinates,

$$H_- = -e^{-i\varphi}[\nabla_\theta - i \cot\theta \, \nabla_\varphi]. \tag{18.13}$$

Taking into account that $v_{-l}(\theta, \varphi) = e^{-il\varphi} F_{-l}(\theta)$, we get from $H_- v_{-l}(\theta, \varphi) = 0$ the differential equation $(\nabla_\theta - \cot\theta l) F_{-l} = 0$. Hence $F_{-l} = C \sin^l \theta$ which means that $-l$ is a simple eigenvalue. By definition of the space $L(j)$, we have $\Lambda v_{-l}(\theta, \varphi) = \lambda_j v_{-l}(\theta, \varphi)$. Substituting $v_{-l}(\theta, \varphi) = e^{-il\varphi} \sin^l \theta$ and using (17.18), we get $\lambda_j = -l(l+1)$.

Next consider the eigenvalue $m = -l+1$. For corresponding eigenfunctions $e^{i(-l+1)\varphi} F_{-l+1}(\theta)$ we have $H_- v_{-l+1}(\theta, \varphi) = C v_{-l}(\theta, \varphi)$ with a $C \in \mathbb{C}$ by Lemma 18.11. Moreover, $C \neq 0$: otherwise, we would have $j = -(l-1)l$ as above. However, this contardicts previous calculation $\lambda_j = -l(l+1)$ since $l \geq 0$. Therefore, we can assume $C = 1$ and get the differential equation $(\nabla_\theta + \cot\theta(-l+1)) F_{-l+1} = F_{-l}$. If the bounded solution exists, it is unique since the solution to the homogeneous equation corresponds to different eigenvalue λ_j. Hence, $-l+1$ also is a simple eigenvalue, etc. ■

Corollary 18.13 *In $D(l)$ there exists a basis $\{F_{lm}(\theta)e^{is\varphi} : m = -l, ..., l\}$.*

Remark 18.14 *The stationary state $\psi(x) = CR_{ln}(r)F_{lm}(\theta)e^{is\varphi}$ is an eigenfunction of the angular momentum $M_3 = \dfrac{i\hbar}{2}\nabla\varphi$. Corresponding eigenvalue is equal to $-m\hbar/2$.*

18.4 Angular Momentum in Spherical Coordinates

We prove (18.13). First, let us rewrite (17.14) as

$$\nabla\psi(r,\theta,\varphi) = e_r\nabla_r\psi + e_\theta\frac{\nabla_\theta\psi}{r} + e_\varphi\frac{\nabla_\varphi\psi}{r\sin\theta} = e_1\nabla_1\psi + e_3\nabla_3\psi + e_3\nabla_3\psi, \tag{18.14}$$

wher $e_1 := (1,0,0)$, etc. Then it is evident geometrically that

$$\begin{cases} e_r = (e_1\cos\varphi + e_2\sin\varphi)\sin\theta + e_3\cos\theta, \\ e_\theta = (e_1\cos\varphi + e_2\sin\varphi)\cos\theta - e_3\sin\theta, \\ e_\varphi = \ e_2\cos\varphi - e_1\sin\varphi. \end{cases} \tag{18.15}$$

Substituting into (18.14), we get

$$\begin{cases} \nabla_1 = \sin\theta\cos\varphi\nabla_r + \cos\theta\cos\varphi\dfrac{\nabla_\theta}{r} - \sin\varphi\dfrac{\nabla_\varphi}{r\sin\theta}, \\ \nabla_2 = \sin\theta\sin\varphi\nabla_r + \cos\theta\sin\varphi\dfrac{\nabla_\theta}{r} + \cos\varphi\dfrac{\nabla_\varphi}{r\sin\theta}, \\ \nabla_3 = \ \cos\theta\nabla_r - \sin\varphi\dfrac{\nabla_\theta}{r}. \end{cases} \tag{18.16}$$

Substituting (18.16) and (17.12) into $H_k = -i(\mathbf{x}\times\nabla_{\mathbf{x}})_k$, we get

$$\begin{cases} H_1 = i(\sin\varphi\nabla_\theta + \cot\theta\cos\varphi\nabla_\varphi) \\ H_2 = i(-\cos\varphi\nabla_\theta + \cot\theta\sin\varphi\nabla_\varphi) \\ H_3 = -i\nabla_\varphi. \end{cases} \tag{18.17}$$

Finally, two first formulas imply (18.13). ■

19 A uniform external Magnetic Field

19.1 Hydrogen Atom

Now let us consider the Hydrogen Atom in an external uniform static magnetic field B with the vector potential $A(\mathbf{x}) = B \times \mathbf{x}/2$. Let us choose the coordinates in such a way that $B = (0, 0, |B|)$. Then $A(\mathbf{x}) = \frac{1}{2}|B|(-x_2, x_1, 0)$. Therefore, we have the *static* Maxwell field with the potentials

$$\left.\begin{array}{l} \phi(\mathbf{x}) := -\dfrac{e}{|\mathbf{x}|}, \\ \\ A(\mathbf{x}) := \dfrac{1}{2}|B|(-\mathbf{x}_2, \mathbf{x}_1, 0) \end{array}\right| \quad \mathbf{x} \in \mathbb{R}^3. \tag{19.1}$$

Then the Schrödinger Eqn (17.1) becomes

$$i\hbar\partial_t\psi(t,\mathbf{x}) = H_B\psi(t,\cdot) := \frac{1}{2\mu}(-i\hbar\nabla_{\mathbf{x}} - \not{e}A(\mathbf{x}))^2\psi(t,\mathbf{x}) - \frac{e^2}{|\mathbf{x}|}\psi(t,\mathbf{x}), \qquad (t,\mathbf{x}) \in \mathbb{R}^4. \tag{19.2}$$

Remark 19.1 *Now (18.6) holds for $e = e_3$:*

$$M_3(t) = \text{const} \tag{19.3}$$

which reflects the axial symmetry of the equation (19.2).

The stationary Schrödinger Eqn (17.8) becomes,

$$\begin{aligned} E_\omega\psi_\omega(\mathbf{x}) = H_B\psi(\mathbf{x}) = & -\frac{1}{2\mu}\hbar^2\Delta\psi_\omega(\mathbf{x}) + i\frac{\hbar\not{e}}{2\mu}[(\nabla_{\mathbf{x}}\cdot A(\mathbf{x}))\psi_\omega(\mathbf{x}) + 2A(\mathbf{x})\cdot\nabla_{\mathbf{x}}\psi_\omega(\mathbf{x})] \\ & -\frac{1}{2\mu}\hbar^2A^2(\mathbf{x})\psi_\omega(\mathbf{x}) - \frac{e^2}{|\mathbf{x}|}\psi_\omega(\mathbf{x}), \qquad \mathbf{x} \in \mathbb{R}^3. \end{aligned} \tag{19.4}$$

Let us note that $\nabla_{\mathbf{x}} \cdot A(\mathbf{x}) \equiv 0$ and $A(\mathbf{x}) \cdot \nabla_{\mathbf{x}} = |B|\nabla_\varphi/2$ where φ is the angular coordinate of the rotation around the vector $e_3 := (0, 0, 1)$, i.e. around B. Then (19.4) becomes

$$\begin{aligned} E_\omega\psi_\omega(\mathbf{x}) = H_B\psi(\mathbf{x}) \quad = \quad & -\frac{1}{2\mu}\hbar^2\Delta\psi_\omega(\mathbf{x}) + i\omega_L\nabla_\varphi\psi_\omega(\mathbf{x}) \\ & -\frac{1}{2\mu}\hbar^2A^2(\mathbf{x})\psi_\omega(\mathbf{x}) - \frac{e^2}{|\mathbf{x}|}\psi_\omega(\mathbf{x}), \qquad \mathbf{x} \in \mathbb{R}^3, \end{aligned} \tag{19.5}$$

where $\omega_L := \hbar\not{e}|B|/(2\mu)$ is the **Larmor Frequency**. Finally, let us assume the field B be small:

$$|B| \ll 1. \tag{19.6}$$

Then we can neglect the term with A^2 in (19.5) and get the equation

$$\begin{aligned} E_\omega\psi_\omega(\mathbf{x}) = H_B^1\psi_\omega(\mathbf{x}) \quad = \quad & -\frac{1}{2\mu}\hbar^2\Delta\psi_\omega(\mathbf{x}) + i\omega_L\nabla_\varphi\psi_\omega(\mathbf{x}) - \frac{e^2}{|\mathbf{x}|}\psi_\omega(\mathbf{x}) \\ = \quad & H\psi_\omega(\mathbf{x}) + i\omega_L\nabla_\varphi\psi_\omega(\mathbf{x}), \qquad \mathbf{x} \in \mathbb{R}^3. \end{aligned} \tag{19.7}$$

Therefore, Theorem 17.4, Corollary 18.13 and (17.32) imply the following theorem.

Theorem 19.2 *i) The Quantum Stationary States ψ_ω of Hydrogen Atom in magnetic field exist for energies $E_\omega = E_{nm} := -R/n^2 + m\omega_L$, where $n = 1, 2, 3...$ and $m = 0, \pm1, ..., \pm(n-1)$. For other energies the states do not exist.*
ii) The eigenfunctions ψ_ω have the form (17.34) in the spherical coordinates.

19.2 A Radial Scalar Potential

Let us consider more general equations of type (19.1) with a static radial external potential $\phi(|x|)$ and the static uniform magnetic field B. Then corresponding eigenvalue problem of type (19.7) becomes

$$E_\omega\psi_\omega(\mathbf{x}) = -\frac{1}{2\mu}\hbar^2\Delta\psi_\omega(\mathbf{x}) + i\omega_L\nabla_\varphi\psi_\omega(\mathbf{x}) + e\phi(|\mathbf{x}|)\psi_\omega(\mathbf{x})$$

$$= H_c\psi_\omega(\mathbf{x}) + i\omega_L\nabla_\varphi\psi_\omega(\mathbf{x}), \qquad \mathbf{x}\in\mathbb{R}^3, \tag{19.8}$$

where H_c the Schrödinger operator with the radial potential. The following theorem can be proved by the same arguments as Theorems 17.4, 19.2.

Theorem 19.3 *i) The Quantum Stationary States ψ_ω of the electron in the static central static electrical and uniform magnetic fields correspond to the energies $E_\omega = E_{lmn}$ of the form $E_{lmn} = E_{ln} + m\omega_L$, where $n = 1, 2, 3...$, $l = 0, 1, ...$ and $m = -l, ..., l$.*
ii) The corresponding eigenfunctions ψ_ω have the following form in the spherical coordinates (cf. (17.34)):

$$\psi_\omega = R_{ln}(r)F_{lm}(\theta)e^{im\varphi}, \tag{19.9}$$

where $F_{lm}(\theta)e^{im\varphi} \in D(l)$.

20 Coupled Maxwell-Schrödinger Equations

Let us determine the dynamics of Maxwell Field in presence of the wave field ψ governed by the Schrödinger Equation. The Lagrangian density of free Maxwell Field is known from (14.7), so we have to modify only the interaction term in (14.7). The interaction term gives the dynamics of Maxwell Field in presence of given charge-current densities (14.7), so it remains to express the densities in the wave field ψ.

On the other hand, we have shown that the interaction from (14.7) term determine uniquely the Lorentz Dynamics (14.10). The Schrödinger Equation (16.22) substitutes the Lorentz Dynamics (14.10). This suggests to identify the Maxwell- Schrödinger interaction with the interaction term from the Lagrangian density $\mathcal{L}_S$ of the Schrödinger Equation (16.22). Namely, we add the Lagrangian density $\mathcal{L}_S$ of the Schrödinger Equation (16.22) to the density $\mathcal{L}_f$ of the free Maxwell field and get the Lagrangian density $\mathcal{L}_{MS}$ of the coupled Maxwell-Schrödinger Equations,

$$\mathcal{L}_{MS}(x,\psi,\nabla\psi) = [i\hbar\nabla_t - e\phi(x)]\psi\cdot\psi - \frac{1}{2\mu}\sum_{k=1}^{3}|(-i\hbar\nabla_k - \not{e}A_k(x))\psi|^2 - \frac{1}{16\pi}\mathcal{F}^{\alpha\beta}\mathcal{F}_{\alpha\beta}. \tag{20.1}$$

Corresponding Euler-Lagrange Equations read,

$$\left\{\begin{array}{l} [i\hbar\nabla_t - e\phi(t,\mathbf{x})]\psi(t,\mathbf{x}) = \dfrac{1}{2\mu}[-i\hbar\nabla_{\mathbf{x}} - \not{e}A(t,\mathbf{x})]^2\psi(t,\mathbf{x}), \\ \\ \dfrac{1}{4\pi}\nabla_\alpha\mathcal{F}^{\alpha\beta}(t,\mathbf{x}) = \left(\begin{array}{ll} \rho := e|\psi(t,\mathbf{x})|^2, & \beta = 0, \\ \\ \dfrac{\mathbf{j}_\beta}{c} := \dfrac{\not{e}}{\mu}[-i\hbar\nabla_\beta - \not{e}A_\beta(t,\mathbf{x})]\psi(t,\mathbf{x})\cdot\psi(t,\mathbf{x}), & \beta = 1,2,3, \end{array}\right) \end{array}\right. \tag{20.2}$$

where the tensor field $\mathcal{F}^{\alpha\beta}$ corresponds to the potentials $\phi(t,\mathbf{x}), A(t,\mathbf{x})$. The system (20.2) describes the dynamics of the wave field ψ in its "own" Maxwell field $\phi(t,\mathbf{x}), A(t,\mathbf{x})$ generated by by the charges and currents of the wave field.

Remark 20.1 *The charge-current densities from (20.2) coincide, up to a factor, with the Noether currents (10.23) corresponding to the group of internal rotations (9.12).*

Now let us introduce static potentials $\phi^{\text{ext}}(t,\mathbf{x})$, $A^{\text{ext}}(t,\mathbf{x})$ of the Maxwell field generated by some external sources. We formalize the introduction through the Lagrangian density

$$\mathcal{L}_{MS}(x,\psi,\nabla\psi) = [i\hbar\nabla_t - e(\phi(x) + \phi^{\text{ext}}(t,\mathbf{x}))]\psi\cdot\psi$$

$$-\frac{1}{2\mu}\sum_{k=1}^{3}|[-i\hbar\nabla_k - \not{e}(A_k(x) + A_k^{\text{ext}}(x))]\psi|^2 - \frac{1}{16\pi}\mathcal{F}^{\alpha\beta}\mathcal{F}_{\alpha\beta}. \tag{20.3}$$

Then corresponding equations read,

$$\left\{\begin{array}{l} [i\hbar\nabla_t - e(\phi(t,\mathbf{x}) + \phi^{\text{ext}}(t,\mathbf{x}))]\psi(t,\mathbf{x}) = \dfrac{1}{2\mu}[-i\hbar\nabla_{\mathbf{x}} - \not{e}(A(t,\mathbf{x}) + A^{\text{ext}}(t,\mathbf{x}))]^2\psi(t,\mathbf{x}), \\ \\ \dfrac{1}{4\pi}\nabla_\alpha\mathcal{F}^{\alpha\beta}(t,\mathbf{x}) = \left(\begin{array}{l} \rho := e|\psi(t,\mathbf{x})|^2, \\ \\ \dfrac{\mathbf{j}_\beta}{c} := \dfrac{\not{e}}{\mu}[-i\hbar\nabla_\beta - \not{e}(A_\beta(t,\mathbf{x}) + A_\beta^{\text{ext}}(t,\mathbf{x}))]\psi(t,\mathbf{x})\cdot\psi(t,\mathbf{x}), \end{array}\right) \end{array}\right. \tag{20.4}$$

20.1 Charge Continuity Equations

The Lagrangian density (20.3) is invariant with respect to the internal rotations (9.12). Furthermore, the densitites $\rho, \mathbf{j}$ from (20.4) coincide with the corresponding Noether currents of the form (10.23)) up to a factor. Therefore, the Noether Theorem II implies

Lemma 20.2 *For any solution to the Schrödinger Equation (20.4), the corresponding charge-current densitites $\rho, \mathbf{j}$ satisfy the continuity equation (11.2).*

Let us prove a more general relation:

Lemma 20.3 *For any two solutions $\psi_1(t,\mathbf{x}), \psi_2(t,\mathbf{x})$ to the Schrödinger equation from (20.4) the following identity holds:*

$$\dot\rho_{12}(t,\mathbf{x}) + \operatorname{div} \mathbf{j}_{12}(t,\mathbf{x}) = 0, \qquad (t,\mathbf{x}) \in \mathbb{R}^4, \tag{20.5}$$

where

$$\begin{cases} \rho_{12}(t,\mathbf{x}) := & e\psi_1(t,\mathbf{x})\overline{\psi}_2(t,\mathbf{x}), \\ \mathbf{j}_{12}(t,\mathbf{x}) := & \dfrac{e}{2\mu}[-i\hbar\nabla_{\mathbf{x}} - \not{e}(A(t,\mathbf{x}) + A^{\rm ext}(t,\mathbf{x}))]\psi_1(t,\mathbf{x})\overline{\psi}_2(t,\mathbf{x}) \\ & + \dfrac{e}{2\mu}[i\hbar\nabla_{\mathbf{x}} - \not{e}(A(t,\mathbf{x}) + A^{\rm ext}(t,\mathbf{x}))]\overline{\psi}_2(t,\mathbf{x})\psi_1(t,\mathbf{x}). \end{cases} \tag{20.6}$$

Remark 20.4 *For $\psi_1 = \psi_2$ the expressions (20.6) become (20.4) by (6.3), and the identity (20.5) becomes (11.2).*

Proof of Lemma 20.3 Let us write (11.2) for ψ_1 and $\overline{\psi}_2$:

$$\left\{ \begin{array}{l} [i\hbar\partial_t - e\phi(\mathbf{x})]\psi_1(t,\mathbf{x}) = \dfrac{1}{2\mu}[-i\hbar\nabla_{\mathbf{x}} - \not{e}(A(t,\mathbf{x}) + A^{\rm ext}(t,\mathbf{x}))]^2\psi_1(t,\mathbf{x}), \\ [-i\hbar\partial_t - e\phi(\mathbf{x})]\overline{\psi}_2(t,\mathbf{x}) = \dfrac{1}{2\mu}[i\hbar\nabla_{\mathbf{x}} - \not{e}(A(t,\mathbf{x}) + A^{\rm ext}(t,\mathbf{x}))]^2\overline{\psi}_2(t,\mathbf{x}) \end{array} \right| \quad (t,\mathbf{x}) \in \mathbb{R}^4. \tag{20.7}$$

Let us multiply first equation by $i\overline{\psi}_2(t,\mathbf{x})$ and add second equation multiplied by $-i\psi_1(t,\mathbf{x})$. Then we get,

$$\begin{aligned} & i\hbar\partial_t\psi_1(t,\mathbf{x})\cdot i\overline{\psi}_2(t,\mathbf{x}) + i\hbar\partial_t\overline{\psi}_2(t,\mathbf{x})\cdot i\psi_1(t,\mathbf{x}) \\ & = \frac{1}{2\mu}[-i\hbar\nabla_{\mathbf{x}} - \not{e}(A(t,\mathbf{x}) + A^{\rm ext}(t,\mathbf{x}))]^2\psi_1(t,\mathbf{x})\cdot i\overline{\psi}_2(t,\mathbf{x}) \\ & + \frac{1}{2\mu}[i\hbar\nabla_{\mathbf{x}} - \not{e}(A(t,\mathbf{x}) + A^{\rm ext}(t,\mathbf{x}))]^2\overline{\psi}_2(t,\mathbf{x})\cdot i\psi_1(t,\mathbf{x}). \end{aligned} \tag{20.8}$$

It is possible to rewrite in the form

$$\begin{aligned} & -\partial_t[\psi_1(t,\mathbf{x})\overline{\psi}_2(t,\mathbf{x})] \\ & = \frac{1}{2\mu}\nabla\cdot\Big([-i\hbar\nabla_{\mathbf{x}} - \not{e}(A(t,\mathbf{x}) + A^{\rm ext}(t,\mathbf{x}))]\psi_1(t,\mathbf{x})\overline{\psi}_2(t,\mathbf{x}) \\ & + [i\hbar\nabla_{\mathbf{x}} - \not{e}(A(t,\mathbf{x}) + A^{\rm ext}(t,\mathbf{x}))]\overline{\psi}_2(t,\mathbf{x})\psi_1(t,\mathbf{x})\Big). \end{aligned} \tag{20.9}$$

■

20.2 The Born Approximation

Let us assume that the own Maxwell fields are small with respect to the external field. Then we can neglect the own field in the first equation of (20.4) and consider the approximate equation

$$[i\hbar\nabla_t - e\phi^{\rm ext}(t,\mathbf{x})]\psi(t,\mathbf{x}) = \frac{1}{2\mu}[-i\hbar\nabla_{\mathbf{x}} - \not{e}A^{\rm ext}(t,\mathbf{x})]^2\psi(t,\mathbf{x}). \tag{20.10}$$

Its solution is an approximation to the wave field ψ from (20.4). Let us solve the equation and substitute the solution ψ into the RHS of the second equation of (20.4):

$$\frac{1}{4\pi}\nabla_\alpha \mathcal{F}^{\alpha\beta}(t,\mathbf{x}) = \left(\begin{array}{l} \rho := e|\psi(t,\mathbf{x})|^2, \\ \\ \dfrac{\mathbf{j}_\beta}{c} := \dfrac{\not{e}}{\mu}[-i\hbar\nabla_\beta - \not{e}A^{\rm ext}_\beta(t,\mathbf{x})]\psi(t,\mathbf{x})\cdot\psi(t,\mathbf{x}), \end{array} \right) \tag{20.11}$$

Then the solution $\mathcal{F}^{\alpha\beta}(t,\mathbf{x})$ gives an approximation to the Maxwell field radiated by the atom. The process of the approximations can be iterated and the obtained fields are known as the *Born approximations*.

21 Atom Radiation and Selection Rules

21.1 The Dipole Radiation

Let us apply the Born approximations to the calculation of the radiation of an atom with the electrostatic potential $\phi^{\rm ext}(t,\mathbf{x}) = \phi^{\rm ext}(\mathbf{x})$. Let us put the atom in a static magnetic field with a vector potential $A^{\rm ext}(\mathbf{x})$. Then (20.10) becomes

$$[i\hbar\nabla_t - e\phi^{\rm ext}(\mathbf{x})]\psi(t,\mathbf{x}) = \frac{1}{2\mu}[-i\hbar\nabla_{\mathbf{x}} - \not{e}A^{\rm ext}(\mathbf{x})]^2\psi(t,\mathbf{x}). \tag{21.1}$$

21.1.1 The dipole approximation of the retarded potentials

Consider the atom in the thermodynamical equilibrium with a thermostate at a fixed temperature $T > 0$. Then the wave function $\psi(t,\mathbf{x})$ admits an eigenfunction expansion

$$\psi(t,\mathbf{x}) = \sum_k c_k(T)\psi_k(\mathbf{x})e^{-i\omega_k t} + \int_0^\infty c_\omega(T)\psi_\omega(\mathbf{x})e^{-i\omega t}d\omega \tag{21.2}$$

Let us analyse the Maxwell field produced by the corresponding charge and current densities from (20.11). The potentials of the field satisfy the Maxwell equations (11.6), (11.9) and their large time asymptotics for bounded $|x|$ is given by the retarded potentials (13.4):

$$\left\{\begin{array}{l} \phi(t,\mathbf{x}) \sim \ \phi_{ret}(t,\mathbf{x}) := \ \displaystyle\int \frac{\rho(t-|\mathbf{x}-\mathbf{y}|/c,\mathbf{y})}{|\mathbf{x}-\mathbf{y}|}d\mathbf{y} \\ \\ A(t,\mathbf{x}) \sim A_{ret}(t,\mathbf{x}) := \dfrac{1}{c}\displaystyle\int \frac{\mathbf{j}(t-|\mathbf{x}-\mathbf{y}|/c,\mathbf{y})}{|\mathbf{x}-\mathbf{y}|}d\mathbf{y} \end{array}\right| \quad t\to\infty, \quad |\mathbf{x}|\le R. \tag{21.3}$$

Let us assume that the atom is located at the point $\mathbf{y} = 0$. Then the densities $\rho(t,\mathbf{y})$, $\mathbf{j}(t,\mathbf{y})$ are localized in a ball $|\mathbf{y}| \le a \ll 1$. Therefore, any macroscopic observation at a distance $|\mathbf{x}| \sim 1$ coincides with a high precision with the *dipole approximation*

$$\left\{\begin{array}{l} \phi(t,\mathbf{x}) \sim \ \dfrac{1}{|\mathbf{x}|}\displaystyle\int_{|\mathbf{y}|\le a} \rho(t-|\mathbf{x}-\mathbf{y}|/c,\mathbf{y})d\mathbf{y} \\ \\ A(t,\mathbf{x}) \sim \dfrac{1}{c|\mathbf{x}|}\displaystyle\int_{|\mathbf{y}|\le a} \mathbf{j}(t-|\mathbf{x}-\mathbf{y}|/c,\mathbf{y})d\mathbf{y} \end{array}\right| \quad t\to\infty, \quad |\mathbf{x}|\le R. \tag{21.4}$$

Let us calculate the charge-current densities corresponding to the wave function (21.2). By (20.11) and (6.3), we have

$$\left\{\begin{array}{l} \rho(t,\mathbf{y}) = e\psi(t,\mathbf{y})\overline{\psi(t,\mathbf{y})}, \\ \\ \mathbf{j}(t,\mathbf{y}) = \Re\left[\left(\dfrac{e}{2\mu}[-i\hbar\nabla_{\mathbf{y}} - \not{e}A^{\rm ext}(\mathbf{y})]\psi(t,\mathbf{y})\right)\overline{\psi(t,\mathbf{y})}\right]. \end{array}\right. \tag{21.5}$$

The oscillatory integral in (21.2) over the continuous spectrum converges to zero for large t and bounded $|\mathbf{y}|$. Hence $\psi(t,\mathbf{y}) \sim \psi_d(t,\mathbf{y}) := \sum_k c_k(T)\psi_k(\mathbf{y})e^{-i\omega_k t}$, $t\to\infty$, for the bounded $|\mathbf{y}|$.

Substituting the asymptotics for $\psi(t,\mathbf{y})$ into (21.5), we get for $t\to\infty$, and bounded $|\mathbf{y}|$:

$$\begin{cases} \rho(t-|\mathbf{x}-\mathbf{y}|/c,\mathbf{y}) \approx \Re\sum_{kk'} a_{kk'}(T)e^{-i(\omega_k-\omega_{k'})(t-|\mathbf{x}-\mathbf{y}|/c)}\psi_k(\mathbf{y})\overline{\psi_{k'}(\mathbf{y})}, \\ \mathbf{j}(t-|\mathbf{x}-\mathbf{y}|/c,\mathbf{y}) \approx \\ \Re\sum_{kk'} A_{kk'}(T)e^{-i(\omega_k-\omega_{k'})t}\Big([-i\hbar\nabla_{\mathbf{y}}-\not{e}A^{\rm ext}(\mathbf{y})]\psi_k(\mathbf{y})e^{-i\omega_k|\mathbf{x}-\mathbf{y}|/c}\Big)\overline{\psi_{k'}(\mathbf{y})}e^{-i\omega_{k'}|\mathbf{x}-\mathbf{y}|/c}. \end{cases}$$

If we substitute the asymptotics into (21.4), we get the spectral expansion of the radiation in the dipole approximation:

$$(21.6)\qquad \left\{\begin{array}{l} \phi(t,\mathbf{x}) \approx \dfrac{1}{|\mathbf{x}|}\Re\displaystyle\sum_{kk'} a_{kk'}(\mathbf{x},T)e^{-i(\omega_k-\omega_{k'})t}, \\ \\ A(t,\mathbf{x}) \approx \dfrac{1}{c|\mathbf{x}|}\Re\displaystyle\sum_{kk'} A_{kk'}(\mathbf{x},T)e^{-i(\omega_k-\omega_{k'})t} \end{array}\right| \quad t\to\infty,\quad |\mathbf{x}|\le R.$$

Corollary 21.1 *The Rydberg-Ritz Combination Principle holds: the spectrum of the atom radiation is contained in the set* $\{\omega_{kk'} := \omega_k - \omega_{k'}\}$.

Further, the limiting amplitudes in (21.6) are given by

$$(21.7)\qquad \begin{cases} a_{kk'}(\mathbf{x},T) = a_{kk'}(T)\displaystyle\int_{|\mathbf{y}|\le a} e^{-i\omega_{kk'}|\mathbf{x}-\mathbf{y}|/c}\psi_k(\mathbf{y})\overline{\psi_{k'}(\mathbf{y})}d\mathbf{y}, \\ \\ A_{kk'}(\mathbf{x},T) \approx b_{kk'}(T)\displaystyle\int_{|\mathbf{y}|\le a} e^{-i\omega_{kk'}|\mathbf{x}-\mathbf{y}|/c}[-i\hbar\nabla_{\mathbf{y}}-\not{e}A^{\rm ext}(\mathbf{y})]\psi_k(\mathbf{y})\overline{\psi_{k'}(\mathbf{y})}d\mathbf{y} \end{cases}$$

with an error of order $\hbar\omega_k/c$ in the last formula.

21.1.2 Selection Rules in the Cylindrical Symmetry

Let us consider the case of a **radial** electrostatic potential $\phi^{\rm ext}(\mathbf{x}) = \phi^{\rm ext}(|\mathbf{x}|)$ and a static **uniform** magnetic field B. Then the vector potential $A^{\rm ext}(\mathbf{x}) = B\times\mathbf{x}/2$. Let us consider a fixed spectral line $\omega_{kk'}\neq 0$ where ω_k resp. $\omega_{k'}$ correponds to the eigenfunction (see (19.9))

$$(21.8)\qquad \psi_\omega = R_{nl}(r)F_{lm}(\theta)e^{im\varphi},\quad \text{resp.}\quad \psi_{\omega'} = R_{n'l'}(r)F_{l'm'}(\theta)e^{im'\varphi}.$$

Let us assume that

$$(21.9)\qquad |\omega_{kk'}|a/c \ll 1$$

which means that the wave length $\lambda_{kk'} := 2\pi c/|\omega_{kk'}| \gg a$.

Theorem 21.2 *Let the condition (21.9) hold,* $\phi^{\rm ext}(\mathbf{x}) = \phi^{\rm ext}(|\mathbf{x}|)$ *and* $A^{\rm ext}(\mathbf{x}) = B\times\mathbf{x}/2$. *Then for the dipole approximations of the limiting amplitudes with* $\omega_k\neq\omega_{k'}$ *we have: i)* $a_{kk'}(\mathbf{x},T)=0$ *and ii)* $A_{kk'}(\mathbf{x},T)\neq 0$ *only if* $l'=l\pm1$ *and* $m'=m,m\pm1$.

Proof Under condition (21.9) the exponent in the integrands of (21.7) is close to a constant $e_{kk'}(x) := \exp(-i\omega_{kk'}\mathbf{x}/c)$ since $|\mathbf{y}|\le a$. In addition, the ball of integration $|\mathbf{y}|\le a$ can be

substituted by the whole space since the eigenfunctions ψ_k, $\psi_{k'}$ are well localized. Therefore, (21.7) becomes

$$\begin{cases} a_{kk'}(\mathbf{x},T) = a_{kk'}(T)e_{kk'}(x)\displaystyle\int \psi_k(\mathbf{y})\overline{\psi_{k'}(\mathbf{y})}d\mathbf{y}, \\ \\ A_{kk'}(\mathbf{x},T) = b_{kk'}(T)e_{kk'}(x)\displaystyle\int [-i\hbar\nabla_{\mathbf{y}} - \not{e}A^{\rm ext}(\mathbf{y})]\psi_k(\mathbf{y})\overline{\psi_{k'}(\mathbf{y})}d\mathbf{y}. \end{cases} \tag{21.10}$$

Now $a_{kk'}(\mathbf{x},T) = 0$ by the orthogonality of different eigenfunctions since we consider $\omega_k \neq \omega_{k'}$. To analyze $A_{kk'}(\mathbf{x},T)$, let us use the identity (20.5) for the solutions $\psi_k(\mathbf{x})e^{-i\omega_k t}$, $\psi_{k'}(\mathbf{x})e^{-i\omega_{k'}t}$ to the equation (20.10). For this Born's approximation we have $A(t,\mathbf{x}) = 0$ hence the formulas (20.6) give the densities

$$\begin{cases} \rho_{kk'}(t,\mathbf{x}) := & e^{-i\omega_{kk'}t}e\psi_k(\mathbf{x})\overline{\psi_{k'}(\mathbf{x})}, \\ \\ \mathbf{j}_{kk'}(t,\mathbf{x}) := & e^{-i\omega_{kk'}t}\Big(\dfrac{e}{2\mu}[-i\hbar\nabla_{\mathbf{x}} - \not{e}A^{\rm ext}(\mathbf{x})]\psi_k(\mathbf{x})\overline{\psi_{k'}(\mathbf{x})} \\ \\ & \qquad + \dfrac{e}{2\mu}[i\hbar\nabla_{\mathbf{x}} - \not{e}A^{\rm ext}(\mathbf{x})]\overline{\psi_{k'}(\mathbf{x})}\psi_k(\mathbf{x})\Big) \end{cases} \tag{21.11}$$

Then (20.5) becomes

$$-i\omega_{kk'}\rho_{kk'}(t,\mathbf{x}) + \operatorname{div}\mathbf{j}_{kk'}(t,\mathbf{x}) = 0, \qquad (t,\mathbf{x}) \in \mathbb{R}^4. \tag{21.12}$$

By partial integration we see that the integral in the second formula of (21.10) is proportional to the integral of $\mathbf{j}_{kk'}(t,\mathbf{x})$. Therefore, it remains to prove

Lemma 21.3

$$\int \mathbf{j}_{kk'}(t,\mathbf{x})d\mathbf{x} = 0, \qquad t \in \mathbb{R}, \tag{21.13}$$

if either $l' \neq l \pm 1$ *or* $m' \neq m, m \pm 1$.

Proof Let us multiply (21.12) by the coodinate $\mathbf{x}^p$, $p = 1,2,3$, and integrate over $\mathbb{R}^3$. Then we get by partial integration,

$$-i\omega_{kk'}\int \mathbf{x}^p\rho_{kk'}(t,\mathbf{x})d\mathbf{x} - \int \mathbf{j}^p_{kk'}(t,\mathbf{x})d\mathbf{x} = 0, \tag{21.14}$$

where $\mathbf{j}^p_{kk'}$ is the p-th component of $\mathbf{j}_{kk'}$. Hence,

$$\int \mathbf{j}^p_{kk'}(t,\mathbf{x})d\mathbf{x} \sim \int \mathbf{x}^p\psi_k(\mathbf{x})\cdot\psi_{k'}(\mathbf{x})d\mathbf{x}. \tag{21.15}$$

Let us rewrite last integral in the spherical coordinates. Then we get by (21.8),

$$\begin{aligned} &\int \mathbf{x}^p\psi_k(\mathbf{x})\cdot\psi_{k'}(\mathbf{x})d\mathbf{x} \\ &= \int_0^\infty R_{nl}(r)\overline{R_{n'l'}(r)}r^3dr\int_S \frac{\mathbf{x}^p}{r}F_{lm}(\theta)e^{im\varphi}\overline{F_{l'm'}(\theta)e^{im'\varphi}}dS. \end{aligned} \tag{21.16}$$

Obviously, the last integral is equal to zero if $m' \neq 0, m \pm 1$. For $l' \neq l \pm 1$ this property is proved in [3, Appendix XXI]. ■

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