

Conservation Laws in Physics

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We briefly review the conservation laws in physics.

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I. INTRODUCTION

A reference frame is defined by a set of operative rules to measure physical quantities.

The same physical phenomenon can be observed from two different reference frames. In order for the two reference frames to be defined, the transformation between the quantities measured in the two frames must be known.

In a given reference frame a phenomenon obeys certain physical laws. A physical law is a relationship which poses conditions on the quantities measured at a given instant.

The frames are said to be equivalent respect to a class of phenomena if:

- a) Any physical situation realizable in one can also be realizable in the other.
- b) The time evolution laws are the same in the two frames.

The equivalence between frames produced by the invariance is an equivalence relationship in the mathematical sense: Given R, R', R'' three frames; R is equivalent to R' , if R is equivalent to R' then R' is equivalent to R ; if R is equivalent to R' and R' is equivalent to R'' then R is equivalent to R'' .

The transformation laws between quantities in equivalent frames form a group:

- a) The identity transformation exists: The one between any frame and itself.
- b) Given any transformation, an inverse transformation exists which is itself an equivalence relationship respect to the class of phenomena in exam.
- c) The product of two equivalence relationships, defined as the application in succession and ordered of two transformations, is still an equivalence relationship.

The equivalence of a class of frames relative to a set of phenomena is called *invariance* of such phenomena relative to the group of transformations between the frames.

Intermezzo

We will skip Statistical Physics and work in *real time* $t = x^0$ ($c = 1$) except in subsections II C on liquid crystals and ?? on liquids where $t \rightarrow -i\beta$ ($\hbar = 1$) according to a Wick rotation that brings Quantum Mechanics into Statistical Mechanics.

Units

We will always use relativistic units with $\hbar = 1, c = 1$. In these units, we have for the elementary charge $e^2/4\pi = 1/137$.

Fourier transform

The tridimensional Fourier transform is

$$f(\mathbf{p}) = \int f(\mathbf{q}) e^{-i\mathbf{q}\cdot\mathbf{p}} d\mathbf{q}, \quad (1.1)$$

$$f(\mathbf{q}) = \int f(\mathbf{p}) e^{i\mathbf{q}\cdot\mathbf{p}} \frac{d\mathbf{p}}{(2\pi)^3}, \quad (1.2)$$

and analogously for the four-dimensional case.

Operators

We will not introduce a different symbol for the operators on the Hilbert space and their eigenvalues. The reader should understand the difference from the context of the various equations introduced.

Indexes

The summation convention always applies to suffixes occurring twice in vector and tensor expressions or to repeated subscript (denoting contravariant components) and superscript (denoting covariant components). Greek indexes run over (3) space (1) time components and Roman indexes run only over (3) space components. Sometimes we use the short hand notation of a subscript comma $_{,\mu}$ or the symbol ∂_μ to denote $\partial/\partial x^\mu$ the partial differentiation with respect to a coordinate. In Section V we will use a subscript semicolon $_{;\mu}$ to denote a covariant derivative.

II. IN CLASSICAL PHYSICS

Consider a classical system of N particles of mass m_i in d dimensions with *positions* $\mathbf{q}_i = (q_i^1, q_i^2, \dots, q_i^d)$ with $i = 1, 2, \dots, N$. We will then have a total of $s = dN$ degrees of freedom. Call $\dot{\mathbf{q}}_i = d\mathbf{q}_i(t)/dt$ the *velocities* of the

N particles where $\mathbf{q}_i = \mathbf{q}_i(t)$ are the N trajectories of the particles. The equation of motion of each particle can be obtained from a variational principle of least action from the following action functional

$$S[\{\mathbf{q}_i\}, \{\dot{\mathbf{q}}_i\}] = \int_0^T \mathcal{L}(\{\mathbf{q}_i\}, \{\dot{\mathbf{q}}_i\}, t) dt, \quad (2.1)$$

where \mathcal{L} is known as the *Lagrangian* function. In order to find agreement between the result of the least action principle $\delta S = 0$ and Newton equations of motion we need to choose

$$\mathcal{L} = \frac{1}{2} \sum_i m_i \dot{\mathbf{q}}_i^2 - U(\{\mathbf{q}_i\}, t) = T - U, \quad (2.2)$$

where U is the potential energy of the system of particles. Where we assumed that the variations $\mathbf{q}_i \rightarrow \mathbf{q}_i + \delta \mathbf{q}_i$ are such that $\delta \mathbf{q}_i(T) = \delta \mathbf{q}_i(0) = 0$. Euler-Lagrange equations of motion that results from the stationary action principle are then

$$\frac{d}{dt} \frac{\partial \mathcal{L}}{\partial \dot{\mathbf{q}}_i} = \frac{\partial \mathcal{L}}{\partial \mathbf{q}_i}. \quad (2.3)$$

A. Classical mechanics [1]

Newton equations of motion are s coupled second order partial differential equations which admit a unique solution only after assigning $2s - 1$ constants that completely determine the initial conditions for $\{\mathbf{q}_i(t_0)\}$ and $\{\dot{\mathbf{q}}_i(t_0)\}$ for a fixed t_0 . These constants are known as *integrals of motion*.

The integrals of motion are usually not amenable of a physical interpretation but only of a mathematical one. In order to make some progress in the physical vision we will see that it is possible to find some physically relevant *conserved quantities* that reflect the *homogeneity* of time and space and the *isotropy* of space. We will then discuss these 3 important conserved quantities next.

Homogeneity of time

Let us consider the conservation law resulting from the *homogeneity of time*. This holds only for a *closed*¹ system for which the Lagrangian does not depend explicitly on time $\mathcal{L} = \mathcal{L}(\{\mathbf{q}_i\}, \{\dot{\mathbf{q}}_i\})$. The total derivative of the Lagrangian can therefore be written

$$\frac{d\mathcal{L}}{dt} = \sum_i \frac{\partial \mathcal{L}}{\partial \mathbf{q}_i} \cdot \dot{\mathbf{q}}_i + \sum_i \frac{\partial \mathcal{L}}{\partial \dot{\mathbf{q}}_i} \cdot \ddot{\mathbf{q}}_i. \quad (2.4)$$

Using the equation of motion (2.3) we find

$$\frac{d\mathcal{L}}{dt} = \sum_i \frac{d}{dt} \frac{\partial \mathcal{L}}{\partial \dot{\mathbf{q}}_i} \cdot \dot{\mathbf{q}}_i + \sum_i \frac{\partial \mathcal{L}}{\partial \dot{\mathbf{q}}_i} \cdot \ddot{\mathbf{q}}_i = \sum_i \frac{d}{dt} \left(\frac{\partial \mathcal{L}}{\partial \dot{\mathbf{q}}_i} \cdot \dot{\mathbf{q}}_i \right). \quad (2.5)$$

Hence we see that the quantity

$$\mathcal{H} = \sum_i \frac{\partial \mathcal{L}}{\partial \dot{\mathbf{q}}_i} \cdot \dot{\mathbf{q}}_i - \mathcal{L}, \quad (2.6)$$

remains constant during the motion of the closed system. This particular integral of motion is called the *energy* of the system. Mechanical systems whose energy is conserved are sometimes called *conservative*.

Since the energy depends linearly on the Lagrangian and the Lagrangian of a non interacting system, i.e. $U = 0$, is additive the same additivity property will be shared with the energy.

Since T in the Lagrangian (2.2) is a quadratic function of the velocities, using Euler theorem on homogeneous functions we have

$$\sum_i \frac{\partial \mathcal{L}}{\partial \dot{\mathbf{q}}_i} \cdot \dot{\mathbf{q}}_i = \sum_i \frac{\partial T}{\partial \dot{\mathbf{q}}_i} \cdot \dot{\mathbf{q}}_i = 2T, \quad (2.7)$$

¹ Note that we here just require that U does not depend explicitly on time, so we accept a system subject to a constant *external* field.

and

$$\mathcal{H} = T + U, \quad (2.8)$$

where T is the *kinetic* energy.

Homogeneity of space

A second conservation law follows from the *homogeneity of space*. By virtue of this homogeneity, the mechanical properties of a closed system are unchanged by any parallel displacement of the entire system in place.

A parallel displacement is a transformation in which every particle in the system is moved by the same amount ϵ . Since the mechanical properties of the system are unaltered by the parallel displacement, the change in \mathcal{L} resulting from an infinitesimal change in the coordinates, the velocities of the particles remaining fixed, must vanish

$$0 = \delta\mathcal{L} = \sum_i \frac{\partial\mathcal{L}}{\partial\mathbf{q}_i} \cdot \epsilon. \quad (2.9)$$

Since ϵ is arbitrary it must be

$$\sum_i \frac{\partial\mathcal{L}}{\partial\mathbf{q}_i} = 0. \quad (2.10)$$

From Euler-Lagrange equation (2.3) we therefore have

$$\frac{d}{dt} \sum_i \frac{\partial\mathcal{L}}{\partial\dot{\mathbf{q}}_i} = 0. \quad (2.11)$$

Thus we conclude that, in a closed mechanical system, the vector

$$\mathcal{P} = \sum_i \frac{\partial\mathcal{L}}{\partial\dot{\mathbf{q}}_i}, \quad (2.12)$$

remains constant during the motion. It is called the *momentum* of the system. The additivity of the momentum is evident. Moreover, unlike the energy, the momentum of the system is equal to the sum of its values $\mathbf{p}_i = m_i\dot{\mathbf{q}}_i$ for individual particles, whether or not the interaction between them can be neglected ².

Eq. (2.10) can be rewritten as

$$\sum_i \mathbf{F}_i = 0 \quad (2.13)$$

where $\mathbf{F}_i = \partial\mathcal{L}/\partial\mathbf{q}_i = -\partial U/\partial\mathbf{q}_i$ is the force acting on particle i . In particular, for a system of only two particles $\mathbf{F}_1 + \mathbf{F}_2 = 0$, i.e. the force exerted by the first particle on the second is equal in magnitude and opposite in direction to that exerted by the second particle on the first. This equality of action and reaction is *Newton third law*.

We can always choose an *inertial* reference frame, i.e. a reference frame moving with constant velocity \mathbf{v} , where the momentum \mathcal{P} is zero. This is the *center of mass* reference frame such that

$$\mathbf{v} = \mathcal{P} / \sum_i m_i, \quad (2.14)$$

where

$$\mathbf{Q} = \sum_i m_i \mathbf{q}_i / \sum_i m_i, \quad (2.15)$$

is the center of mass point.

² Note that some components of the momentum vector \mathcal{P} may be conserved even in the presence of an external field if U does not depend explicitly on all the Cartesian coordinates. The mechanical properties of the system are evidently unchanged by a displacement along the axis of a coordinate which does not appear in the potential, and so the corresponding component of the momentum is conserved.

Isotropy of space

Let us now derive the conservation law which follows from the *isotropy of space*. This isotropy means that the mechanical properties of a closed system do not vary when it is rotated as a whole in any manner in space. Let us therefore consider an infinitesimal rotation of the system, and obtain the condition for the Lagrangian to remain unchanged.

We shall use the vector $\delta\phi$ of the infinitesimal rotation, whose magnitude is the angle of rotation $\delta\phi$, and whose direction is that of the axis of rotation (the direction of rotation being that of a right-handed screw driven along $\delta\phi$).

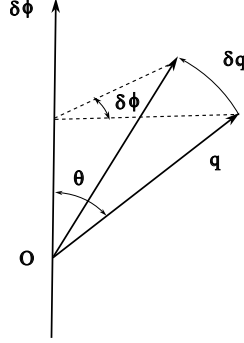


FIG. 1. Pictorial view of the angular velocity vector $\delta\phi/\delta t$. We see how $\delta\mathbf{q} = \delta\phi \times \mathbf{q}$.

Let us find, first of all, the resulting increment in the radius vector from an origin on the axis to any particle in the system undergoing rotation. The linear displacement of the end of the radius vector is related to the angle by $|\delta\mathbf{q}| = r \sin \theta \delta\phi$ as shown in Fig. 1. The direction of $\delta\mathbf{q}$ is perpendicular to the plane of \mathbf{q} and $\delta\phi$. Hence $\delta\mathbf{q} = \delta\phi \times \mathbf{q}$. When the system is rotated, not only the radius vectors but also the velocities of the particles change direction, and all vectors are transformed in the same manner. The velocity increment relative to a fixed system of coordinates is $\delta\dot{\mathbf{q}} = \delta\phi \times \dot{\mathbf{q}}$. If these expressions are substituted in the condition that the Lagrangian is unchanged by the rotation

$$\begin{aligned}
 0 = \delta\mathcal{L} &= \sum_i \left(\frac{\partial\mathcal{L}}{\partial\mathbf{q}_i} \cdot \delta\mathbf{q}_i + \frac{\partial\mathcal{L}}{\partial\dot{\mathbf{q}}_i} \cdot \delta\dot{\mathbf{q}}_i \right) \\
 &= \sum_i (\dot{\mathbf{p}}_i \cdot \delta\phi \times \mathbf{q}_i + \mathbf{p}_i \cdot \delta\phi \times \dot{\mathbf{q}}_i) \\
 &= \delta\phi \cdot \sum_i (\mathbf{q}_i \times \dot{\mathbf{p}}_i + \dot{\mathbf{q}}_i \times \mathbf{p}_i) \\
 &= \delta\phi \cdot \frac{d}{dt} \sum_i \mathbf{q}_i \times \mathbf{p}_i.
 \end{aligned} \tag{2.16}$$

Since $\delta\phi$ is arbitrary, it follows that $(d/dt) \sum_i \mathbf{q}_i \times \mathbf{p}_i = 0$, and we conclude that the vector

$$\mathcal{M} = \sum_i \mathbf{q}_i \times \mathbf{p}_i, \tag{2.17}$$

called the *angular momentum* of the system, is conserved in the motion of a closed system³. Like the linear momentum \mathcal{P} it is additive, whether or not $U = 0$.

We immediately see that the angular momentum depends on the choice of origin except when the system is at rest as a whole, i.e. $\mathcal{P} = 0$. It is also easy to see that

$$\mathcal{M} = \mathcal{M}' + \mathcal{Q} \times \mathcal{P}, \tag{2.18}$$

where \mathcal{M}' is the angular momentum measured in the center of mass reference frame, i.e. the *intrinsic angular momentum*.

³ The law of conservation may hold in a more restricted form even for a system in an external field. It is evident from the above derivation that the component of angular momentum along an axis about which the field is symmetrical is always conserve, for the mechanical properties of the system are unaltered by any rotation about that axis. Here, of course, the angular momentum must be defined relative to an origin lying on the axis.

B. Fluid mechanics [2]

Fluid dynamics concerns itself with the study of the motion of fluids (liquids and gases). Since the phenomena considered in fluid dynamics are macroscopic, a fluid is regarded as a continuous medium. Therefore when we speak of the “point” of a fluid (or of an infinitesimal volume of it) we mean not a single molecule of the fluid but a volume element still containing very many molecules but yet small compared with the volume of the whole fluid.

A mathematical description of the state of a moving fluid consists in specifying the fluid velocity $\mathbf{v} = \mathbf{v}(t, \mathbf{x})$ and any two thermodynamic functions pertaining to the fluid, for instance the pressure $p = p(t, \mathbf{x}, t)$ and the density $\rho = \rho(t, \mathbf{x})$, from which one can determine all other thermodynamic quantities. These 5 quantities are functions of the coordinates $\mathbf{x} = (x, y, z)$ and of time t . Once again we stress that a point \mathbf{r} in space at a given time t refers to a fixed point and not to specific particles of the fluid.

The conservation laws will allow us to determine some fundamental equations of fluid dynamics

Conservation of matter

We consider some volume Ω of space. The mass of fluid in this volume is $\int_{\Omega} \rho d^3\mathbf{x}$. The total mass of fluid flowing out of the volume in unit time is $\oint_{\partial\Omega} \rho \mathbf{v} \cdot d^2\mathbf{S}$ with $d^2\mathbf{S}$ a vector whose magnitude represents the area of an infinitesimal element of the surface $\partial\Omega$ bounding Ω (its frontier), whose direction points along the outward normal to such element. Clearly the decrease, per unit time, in the mass of the fluid in the volume Ω can be written as $-(\partial/\partial t) \int_{\Omega} \rho d^3\mathbf{x}$. So we must have

$$\frac{\partial}{\partial t} \int_{\Omega} \rho d^3\mathbf{x} = - \oint_{\partial\Omega} \rho \mathbf{v} \cdot d^2\mathbf{S} = - \int_{\Omega} \nabla(\rho \mathbf{v}) d^3\mathbf{x}, \quad (2.19)$$

where in the last equality we used Gauss theorem. Since this equation must hold for any Ω , it must be

$$\frac{\partial \rho}{\partial t} + \nabla(\rho \mathbf{v}) = 0. \quad (2.20)$$

This is known as the *equation of continuity*. The vector $\mathbf{j} = \rho \mathbf{v}$ is called the *mass flux density*.

Euler equation

Let us consider some volume Ω in the fluid. The total force acting on this volume is equal to $-\oint_{\partial\Omega} p d^2\mathbf{S}$. Transforming it to a volume integral $-\oint_{\partial\Omega} p d^2\mathbf{S} = -\int_{\Omega} \nabla p d^3\mathbf{x}$ we see that the fluid surrounding any volume $d^3\mathbf{x}$ exerts on that element a force $-d^3\mathbf{x} \nabla p$.

We can then write down the equation of motion of a volume element of the fluid by equating the force $-\nabla p$ to the product of the mass per unit volume, ρ , and the acceleration, $d\mathbf{v}/dt$

$$\rho \frac{d\mathbf{v}}{dt} = -\nabla p. \quad (2.21)$$

Making the total time derivative explicit ⁴ and dividing by ρ

$$\frac{\partial \mathbf{v}}{\partial t} + (\mathbf{v} \cdot \nabla) \mathbf{v} = -\frac{1}{\rho} \nabla p. \quad (2.22)$$

This is known as *Euler equation* and was first obtained by L. Euler in 1755. In deriving this equation we have taken no account of processes of energy dissipation, which may occur in a moving fluid in consequence of internal friction (viscosity) in the fluid and heat exchange between different parts of it. Such fluids are said to be *ideal*.

The absence of heat exchange between different parts of the fluid (and also, of course, between the fluid and bodies adjoining it) means that the motion is *adiabatic* throughout the fluid. Thus the motion of an ideal fluid must necessarily be supposed adiabatic.

⁴ The total derivative d/dt in this context is also called *substantial derivative* to emphasize its connection with the moving substance.

In adiabatic motion the entropy per unit mass $s = s(t, \mathbf{x})$ remains constant, $ds/dt = 0$. Or, making the total time derivative explicit

$$\frac{\partial s}{\partial t} + (\mathbf{v} \cdot \nabla)s = 0. \quad (2.23)$$

Using the continuity equation (2.20) we can rewrite this equation as

$$\frac{\partial \rho s}{\partial t} + \nabla(\rho s \mathbf{v}) = 0, \quad (2.24)$$

where the product $\rho s \mathbf{v}$ is the *entropy flux density*.

If the entropy is constant throughout the volume of the system at some initial instant, it will remain constant at all later times, i.e. $s = \text{constant}$. In this case the motion is said *isentropic*.

From the thermodynamic relation $dw = Tds + (1/\rho)dp$, where w is the enthalpy per unit mass, follows that if s is constant then $dw = (1/\rho)dp$ and so $(\nabla p)/\rho = \nabla w$. Then Euler equation can be rewritten as

$$\frac{d\mathbf{v}}{dt} = \frac{\partial \mathbf{v}}{\partial t} + (\mathbf{v} \cdot \nabla)\mathbf{v} = -\nabla w, \quad (2.25)$$

or ⁵

$$\frac{\partial \mathbf{v}}{\partial t} - \mathbf{v} \times (\nabla \times \mathbf{v}) = -\nabla \left(w + \frac{1}{2}v^2 \right). \quad (2.26)$$

Bernoulli equation

Fluid dynamics is simplified in the case of *steady flow*, i.e. one in which the velocity is constant in time at any point occupied by the fluid. In other words $\partial \mathbf{v} / \partial t = 0$.

A *streamline* is a line such that its tangent at any point gives the direction of the velocity at that point of the fluid. It is determined by the following system of differential equations

$$\frac{dx}{v_x} = \frac{dy}{v_y} = \frac{dz}{v_z}, \quad (2.27)$$

so that for example $dy/dx = v_y/v_x$. In steady flow the streamline does not vary with time, and coincides with the path of a fluid point in space. In non-steady flow this coincidence no longer occurs: the tangent to the streamline gives the direction of the velocity of a fluid point at a point in space at that instant, whereas the tangent to the path gives the direction of the velocity of a fluid point at various times.

Taking the scalar product of Eq. (2.26) with the unit vector ℓ tangent to the streamline at each point we find

$$\frac{\partial}{\partial \ell} \left(\frac{1}{2}v^2 + w \right) = 0. \quad (2.28)$$

since $\ell \propto \mathbf{v}$. We then conclude that

$$\frac{1}{2}v^2 + w = \text{constant along a streamline.} \quad (2.29)$$

This is called *Bernoulli equation* and was derived for an incompressible fluid (see below) in 1738 by D. Bernoulli. In this equation the constant takes different values for different streamlines, in general.

Conservation of circulation

The integral

$$C = \oint \mathbf{v} \cdot d\ell, \quad (2.30)$$

⁵ Here we used the formula $\frac{1}{2}\nabla v^2 = \mathbf{v} \times (\nabla \times \mathbf{v}) + (\mathbf{v} \cdot \nabla)\mathbf{v}$ which follows from the definition of the cross product $(\mathbf{A} \times \mathbf{B})_i = \epsilon_{ijk} \mathbf{A}_j \mathbf{B}_k$, where a sum is subtended on repeated indexes, and from the properties of the contraction of two Levi-Civita tensors $\epsilon_{ijk} \epsilon_{ilm} = \delta_{jl} \delta_{km} - \delta_{jm} \delta_{kl}$ where δ is the Kronecker delta.

taken along some closed contour, is called the *velocity circulation* round the contour.

Let us consider a closed contour drawn in the fluid at some instant. We suppose it to be a “fluid contour”, i.e. composed of points that lie on the fluid. In the course of time these points move about, and the contour moves with them. Let us investigate what happens to the velocity circulation. In other words, let us calculate the time derivative of C

$$\begin{aligned}\frac{dC}{dt} &= \frac{d}{dt} \oint \mathbf{v} \cdot \delta \mathbf{x} \\ &= \oint \frac{d\mathbf{v}}{dt} \cdot \delta \mathbf{x} + \oint \mathbf{v} \cdot \frac{d\delta \mathbf{x}}{dt} \\ &= \oint \frac{d\mathbf{v}}{dt} \cdot \delta \mathbf{x} \\ &= - \oint (\nabla w) \cdot \delta \mathbf{x} = 0,\end{aligned}\tag{2.31}$$

where in the first equality we replaced $d\ell$ with $\delta \mathbf{x}$, in the third equality we used the fact that $\mathbf{v} \cdot d\delta \mathbf{x}/dt = \mathbf{v} \cdot \delta \mathbf{v} = \delta(v^2/2)$, and in the fourth equality we used Euler equation (2.25) for an ideal fluid⁶. We have thus reached the conclusion that, in an ideal fluid, the velocity circulation round a closed “fluid” contour is constant in time. This is the *law of conservation of circulation* also known as *Kelvin theorem* (1869).

By Stokes theorem

$$\oint_{\mathcal{C}} \mathbf{v} \cdot d\ell = \int_{\mathcal{S}} \nabla \times \mathbf{v} \cdot d^2 \mathbf{S} = \text{constant},\tag{2.32}$$

where \mathcal{S} is any surface of the fluid with \mathcal{C} as its frontier, i.e. the loop $\mathcal{C} = \partial \mathcal{S}$. The vector $\nabla \times \mathbf{v}$ is often called the *vorticity* of the fluid flow at a given point. For an infinitesimal loop \mathcal{C} , $\int_{\mathcal{S}} \nabla \times \mathbf{v} \cdot d^2 \mathbf{S} \approx \delta \mathbf{S} \cdot \nabla \times \mathbf{v} = \text{constant}$, which may be pictorially interpreted as the fact that the vorticity moves with the fluid.

Example in atomospherical science

Extract from the course 302 “Atmospherical Science” by Walter Robinson held at Urbana/Champaign during Fall 1992 [13].

In 2007 the Nobel Peace Prize was awarded to the Intergovernmental Panel on Climate Change (IPCC) and former US Vice President Al Gore Jr., the Norwegian Nobel Committee called special attention to their efforts to obtain and disseminate greater knowledge concerning man-made climate changes and the steps that need to be taken to counteract those changes. According to the IPCC, there is a real danger that the climate changes may also increase the danger of war and conflict, because they will place already scarce natural resources, not least drinking water, under greater pressure and put large population groups to flight from drought, flooding, and other extreme weather conditions [14].

In *dynamic meteorology* one applies the fundamental principles of physics to understand and predict the *motion* of the atmosphere. Focusing on the motions of the atmosphere, this subject does *not* address the interactions of electromagnetic radiation or the chemistry with the atmosphere or the microscopic processes involved in the formation of precipitation [15].

Consider a velocity profile \mathbf{u} of the atmosphere. Its *circulation* is defined as in Eq. (2.30).

To study the dynamics of *smoke rings* we may use the momentum equation in an inertial frame and neglect friction (assuming a negligible viscosity)

$$\frac{d\mathbf{u}}{dt} = -g\hat{\mathbf{z}} - \frac{\nabla P}{\rho},\tag{2.33}$$

where g is the gravity constant, ρ is the density of the air, and p is the atmospheric pressure. We then find

$$\frac{dC}{dt} = - \oint \frac{\nabla p}{\rho} \cdot d\ell = - \oint \frac{dp}{\rho}.\tag{2.34}$$

⁶ Here we assume also that the ideal fluid is isentropic. More generally it is just necessary that a one-to-one relation between p and ρ exists, then $-(1/\rho)\nabla p$ in Eq. (2.22) can be written as a gradient of some function.

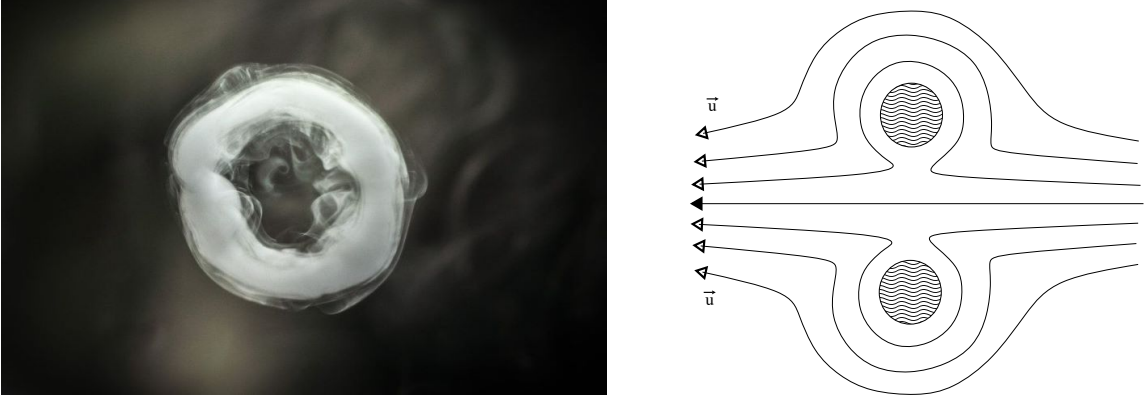


FIG. 2. Vertical section cutting a smoke ring along its diameter and the velocity profile of the air. The smoke is in the wavy regions.

In an ideal incompressible fluid ρ is constant and we find that $dC/dt = 0$, i.e. C is a constant. This is also known as Kelvin circulation theorem that holds more generally for an ideal fluid with $p = p(\rho)$ or $\rho = \rho(p)$ (see Footnote 6).

In Fig. 2 we show a vertical section cutting a smoke ring along its diameter and the velocity profile of the air. From the close up of Fig. 3 we can say that $C = 2\pi r\bar{u}$ with r the internal radius of the smoke torus and \bar{u} the air velocity at the torus surface. Since C is constant as the smoke ring evolves in time its final fate is to disappear with $R \rightarrow \infty$, the ring radius, and $r \rightarrow 0$, the torus internal radius. So that we conclude that the speed of the air at the torus surface must

$$\bar{u} \rightarrow \infty. \quad (2.35)$$

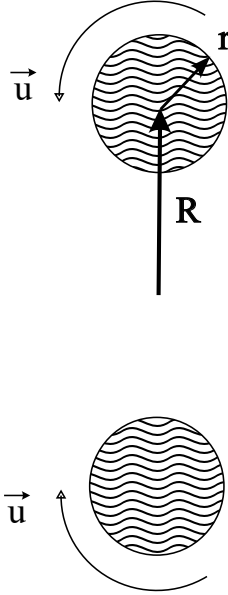


FIG. 3. Close up of the vertical section cutting a smoke ring along its diameter. R is the outer radius of the smoke ring torus and r its inner radius. The velocity \mathbf{u} at the torus surface has magnitude \bar{u} .

Incompressible fluids

Many times the flow of liquids can be regarded as occurring at constant density, i.e. $\rho = \text{constant}$. In other words, there is no noticeable expansion or compression of the fluid in such cases. We then speak of *incompressible flow*.

C. Elasticity [3]: mechanics of liquid crystals [4]

Liquid crystals are, macroscopically, anisotropic fluids. Their study requires a coalition between fluid mechanics and elasticity theory.

Nematics

The *nematic liquid crystals* or *nematics* are substances which in the undeformed state are both macroscopically and microscopically homogeneous. The anisotropy of the medium is due only to the anisotropic spatial orientation of the molecules. The great majority of known nematics belong to the simplest type, in which the anisotropy is fully defined by specifying at each point in the medium a unit vector \mathbf{n} along the particular direction. \mathbf{n} is called the *director*. The quantities \mathbf{n} and $-\mathbf{n}$ are physically equivalent, and so only a particular axis is distinguished, the two opposite directions along it being equivalent. The properties of these nematics in each volume element are invariant under space inversion (a change in sign of all coordinates).

The state of the nematics is thus described by specifying at each point, together with the usual quantities for a liquid (density ρ , pressure p , temperature T , velocity \mathbf{v} , ...), the director \mathbf{n} . All these appear as unknown functions of coordinates and time.

In equilibrium, a nematic at rest under no external forces is homogeneous, with \mathbf{n} constant throughout its volume. In a deformed nematic, the direction of \mathbf{n} varies slowly in space, i.e. the characteristic dimensions of the deformation are much greater than molecular dimensions, so that the derivatives $\partial n_i / \partial x_k \ll 1$.

Here it will be more convenient to relate all thermodynamic quantities to unit volume of the deformed body and not of the undeformed body. Then the free energy density F of a nematic substance is made up of the free energy $F_0(\rho, T)$ of the undeformed nematic and the deformation energy F_d . The latter is given by an expression quadratic in the derivatives of \mathbf{n} , its most general form being

$$F_d = F - F_0 = \frac{1}{2} [K_1(\nabla \mathbf{n})^2 + K_2(\mathbf{n} \cdot \mathbf{curl} \mathbf{n})^2 + K_3(\mathbf{n} \times \mathbf{curl} \mathbf{n})^2]. \quad (2.36)$$

For the unit vector $\mathbf{n}(\mathbf{x})$ since $\nabla \mathbf{n}^2 = 0$, then $\mathbf{n} \times \mathbf{curl} \mathbf{n} = -(\mathbf{n} \cdot \nabla) \mathbf{n}$, and so the last term in Eq. (2.36) can be written in the equivalent form $\frac{1}{2} K_3 [(\mathbf{n} \cdot \nabla) \mathbf{n}]^2$.

The three quadratic combinations of derivatives in (2.36) are independent. Each can be different from zero when the other two are not. The condition for the undeformed state to be stable is therefore that all three coefficients K_1, K_2, K_3 (functions of temperature and density) be positive. We call these the *elastic moduli* or *Frank moduli* of the nematic.

Deformations in which only one of the quantities $\nabla \mathbf{n}$, $\mathbf{n} \cdot \mathbf{curl} \mathbf{n}$, and $\mathbf{n} \times \mathbf{curl} \mathbf{n}$ is non zero are called respectively *plays*, *twists*, and *bends*. In general, of course, the deformation of a nematic includes all three kinds simultaneously.

In absence of external interactions, the equilibrium state that produces the minimum of the deformation free energy (2.36) is then

$$\mathbf{n} = \text{constant}. \quad (2.37)$$

Cholesterics

Cholesteric liquid crystals or *cholesterics* differ from nematics in that there is no center of inversion among their symmetry elements. The directions \mathbf{n} and $-\mathbf{n}$ of the director remain equivalent.

The absence of a center of symmetry has the result that the free energy of deformation may contain a term linear in the pseudoscalar $\mathbf{n} \cdot \mathbf{curl} \mathbf{n}$. The general form of the free energy may be written as

$$F_d = \frac{1}{2} [K_1(\nabla \mathbf{n})^2 + K_2(q + \mathbf{n} \cdot \mathbf{curl} \mathbf{n})^2 + K_3(\mathbf{n} \times \mathbf{curl} \mathbf{n})^2], \quad (2.38)$$

where q is a parameter having dimensions of reciprocal length. This difference respect to the nematics case (2.36) causes a fundamental change in the nature of the equilibrium state of the medium in absence of external interactions: it is no longer uniform in space, $\mathbf{n} = \text{constant}$, as in nematics, but

$$\nabla \mathbf{n} = 0, \quad \mathbf{n} \cdot \mathbf{curl} \mathbf{n} = -q, \quad \mathbf{n} \times \mathbf{curl} \mathbf{n} = 0. \quad (2.39)$$

The free energy of (2.38) then has its minimum value of zero. The solution of these equations is

$$n_x = \cos qz, \quad n_y = \sin qz, \quad n_z = 0. \quad (2.40)$$

This *helicoidal* structure can be regarded as the result of twisting about the z axis a nematic medium originally oriented with $\mathbf{n} = \text{constant}$ in one direction in the xy plane.

Smectics

According to the accepted terminology, *smectic liquid crystals* or *smectics* comprise anisotropic liquids with various layer structures. At least some of these have a microscopic molecular density function that depends on only one coordinate (z , say) and is periodic in that coordinate $\rho = \rho(z)$. A body with density function $\rho(z)$ may be considered as consisting of equidistant plane layers with free relative movement. In each layer, the molecular centers of mass are arranged randomly, and in this sense each of the two-dimensional liquids, but the liquid layers may be either isotropic or not. This difference may be due to the nature of the ordered orientation of molecules in the layers. In the simplest case, the anisotropy of the orientation distribution is specified only by the direction of \mathbf{n} , say the direction of the longest axis of the molecule. If this direction is at right angle to the plane of the layers, then the latter are isotropic, so that the z axis is an axis of symmetry in the body, this appears to be the structure of what are called *smectics A*. If the direction of \mathbf{n} is oblique to the xy plane, that plane contains a preferred direction, and there is no axial symmetry. This appears to be the structure of what are called *smectics B*.

III. IN QUANTUM PHYSICS [5]

In quantum mechanics the invariance respect to a change of reference frame is defined as follows:

- a) The possible states in the two frames are the vectors of a same Hilbert space. The observables are the same. The transformation law is a mapping of the Hilbert space onto itself.
- b) Starting from the same initial state the time evolution is the same in the two frames.

The invariance transformations are a group. So an invariance transformation is a *realization* of the group on an Hilbert space.

Let $|a\rangle$ be a state, in a certain frame, defined by the simultaneous measure of a complete set of commuting observables. Any vector of the form $x_a|a\rangle$ where x_a is an arbitrary phase factor, is an eigenstate of the same observables with the same eigenvalues. So it represents the same physical state. The phase is not observable. A measurement on $|a\rangle$ means to observe the probability that $|a\rangle$ contains a state $|b\rangle$ defined by the measure instruments. What one measures is

$$P_{ab} = |\langle b|a\rangle|^2, \quad (3.1)$$

where the phases x_a and x_b cancel. A vector of the Hilbert space modulo a phase is called a “ray” of the Hilbert space and will be denoted $|\{a\}\rangle$.

Theorem III.1 (Wigner). *Given a bijective transformation between rays in a Hilbert space $|\{s\}\rangle \rightarrow |\{s'\}\rangle$ such that*

$$|\langle\{s'_2\}|\{s'_1\}\rangle|^2 = |\langle\{s_2\}|\{s_1\}\rangle|^2 \quad \forall |\{s_1\}\rangle, |\{s_2\}\rangle \quad (3.2)$$

it is always possible to choose the phases in such a way that the transformation is realized on the Hilbert space vectors as a unitary or antiunitary transformation.

Proof. We will prove Wigner theorem in 3 steps:

1. Let $|e_n\rangle$ be an orthonormal complete base of the Hilbert space and let $|\{e_n\}\rangle$ be the correspondent rays. The transformed rays are orthonormal

$$\langle e_i|e_j\rangle = \delta_{ij} \implies |\langle\{e'_i\}|\{e'_j\}\rangle|^2 = \delta_{ij} \quad (3.3)$$

Let us choose in an arbitrary way a set of phases on the rays $|\{e'_i\}\rangle$, i.e. a set of vectors $|e'_i\rangle$ that represent the states. Then

$$\langle e'_i|e'_j\rangle = \delta_{ij}, \quad (3.4)$$

The set of vectors so obtained is also a complete base of the Hilbert space. In fact, if there exists a vector $|v'\rangle$ such that $\langle v'|v'\rangle \neq 0$ and $\langle v'|e'_n\rangle = 0 \quad \forall n$, then, by hypothesis, there would exist a vector $|v\rangle$ such that $\langle v|v\rangle \neq 0$ and $\langle v|e_n\rangle = 0 \quad \forall n$, against the hypothesis of completeness of the base $|e_n\rangle$.

2. Let $|F_k\rangle = |e_1\rangle + |e_k\rangle$. The generic representative of the transformed ray $|\{F'_k\}\rangle$ will be

$$|F'_k\rangle = x_k(|e'_1\rangle + y_k|e'_k\rangle), \quad (3.5)$$

with x_k and y_k phases factors. In fact

$$|\langle F_k | e_n \rangle| = \delta_{n1} + \delta_{nk} \implies |\langle F'_k | e'_n \rangle| = \delta_{n1} + \delta_{nk}. \quad (3.6)$$

Next I can define the following S transformation

$$|Se_1\rangle = |e'_1\rangle \quad |Se_k\rangle = y_k|e'_k\rangle \quad (3.7)$$

$$|SF_k\rangle = \frac{1}{x_k}|F'_k\rangle = |e'_1\rangle + y_k|e'_k\rangle. \quad (3.8)$$

With this choice

$$|SF_k\rangle = |Se_1\rangle + |Se_k\rangle. \quad (3.9)$$

In other words we realized the transformation S as a linear transformation on vectors of kind $|F_k\rangle$. Let us next extend this construction to all vectors of the Hilbert space.

3. Consider a generic vector

$$|v\rangle = \sum_n a_n |e_n\rangle. \quad (3.10)$$

Let us assume, without loss of generality, a_1 real. The correspondent ray $|\{v\}\rangle$ will be transformed into a ray $|\{v'\}\rangle$ with the following generic representative

$$|v'\rangle = \sum_n a'_n |e'_n\rangle, \quad (3.11)$$

and since by hypothesis

$$|\langle v | e_n \rangle|^2 = |\langle v' | e'_n \rangle|^2, \quad (3.12)$$

we have

$$|a'_n| = |a_n|. \quad (3.13)$$

We define

$$|Se_1\rangle = |e'_1\rangle, \quad (3.14)$$

$$|Se_n\rangle = y_n |e'_n\rangle \quad \forall n \neq 1, \quad (3.15)$$

with y_n some phase factors, so that for any vector belonging to the transformed ray $|\{v'\}\rangle$

$$|v'\rangle = x \left\{ a_1 |Se_1\rangle + \sum_{n=2}^{\infty} \frac{a'_n}{y_n} |Se_n\rangle \right\}, \quad (3.16)$$

with x a phase factor. We then define

$$|Sv\rangle = \frac{1}{x} |v'\rangle. \quad (3.17)$$

By hypothesis it must be

$$|\langle F_k | v \rangle|^2 = |a_1 + a_k|^2 = |\langle SF_k | Sv \rangle|^2 = \left| a_1 + \frac{a'_k}{y_k} \right|^2. \quad (3.18)$$

Since we also have $|a_k| = |a'_k|$ we require

$$\mathbf{Re}(a_1 a_k) = \mathbf{Re}\left(a_1 \frac{a'_k}{y_k}\right). \quad (3.19)$$

Then there are only two possibilities:

- i. $a_k = a'_k/y_k$
- ii. $a_k = (a'_k/y_k)^*$

or

- i. $|Sv\rangle = S(\sum_n a_n |e_n\rangle) = \sum_n a_n |Se_n\rangle$
- ii. $|Sv\rangle = S(\sum_n a_n |e_n\rangle) = \sum_n a_n^* |Se_n\rangle$

In the first case the operator S is linear, in the second is antilinear. We also have

- i. $\langle Sv_1 | Sv_2 \rangle = \langle v_1 | v_2 \rangle \quad \forall |v_1\rangle, |v_2\rangle$
- ii. $\langle Sv_1 | Sv_2 \rangle = \langle v_2 | v_1 \rangle \quad \forall |v_1\rangle, |v_2\rangle$

In the first case S is unitary, in the second it is antiunitary.

□

A. Invariance and time evolution

The requirement b) for invariance tells us that the evolution of the transformed must coincide with the transformation of the evolved

$$U(t, t') S(t') |\psi\rangle = S(t) U(t, t') |\psi\rangle, \quad (3.20)$$

where $U(t, t')$ is the time evolution operator. Since $|\psi\rangle$ is arbitrary we must have

$$S^\dagger(t) U(t, t') S(t') = U(t, t'). \quad (3.21)$$

If the Hamiltonian H is independent of time

$$U(t, t') = e^{-iH(t-t')}, \quad (3.22)$$

and we require

$$S(t) = e^{-iH(t-t')} S(t') e^{iH(t-t')}. \quad (3.23)$$

B. Galilean relativity

We require invariance under translations, rotations, and velocity transformations for pointwise non relativistic particles.

Spatial translations

Let us consider a reference frame R' translated by \mathbf{a} relative to the frame R . If the spatial translations are a symmetry of the system it must exist a unitary transformation $U(\mathbf{a})$ which relates the dynamical variables \mathbf{q}' and \mathbf{p}' in R' to the variables \mathbf{q} and \mathbf{p} in R . The transformation law must be

$$\mathbf{q}' = \mathbf{q} - \mathbf{a}, \quad (3.24)$$

$$\mathbf{p}' = \mathbf{p}. \quad (3.25)$$

It is easy to see that the unitary operator exists and is

$$U(\mathbf{a}) = e^{i\mathbf{a} \cdot \mathbf{p}}. \quad (3.26)$$

Since the transformation is unitary the commutation relations do not change

$$[q'_i, p'_j] = [q_i, p_j] = i\delta_{ij}, \quad (3.27)$$

$$[q'_i, q'_j] = [q_i, q_j] = 0, \quad (3.28)$$

$$[p'_i, p'_j] = [p_i, p_j] = 0, \quad (3.29)$$

where $\mathbf{q} = U(\mathbf{a})^\dagger \mathbf{q} U(\mathbf{a})$ and $\mathbf{p} = U(\mathbf{a})^\dagger \mathbf{p} U(\mathbf{a})$. Moreover from Hadamard lemma (A11) follows immediately that Eqs. (3.24)-(3.25) are satisfied.

The invariance of the time evolution between two frames R and R' imposes

$$U^\dagger(\mathbf{a}, t) e^{-iH(t-t')} U(\mathbf{a}, t') = e^{-iH(t-t')}, \quad (3.30)$$

which means

$$[\mathbf{p}, H] = 0. \quad (3.31)$$

In other words, the momentum is a constant of motion. We can also write

$$\frac{\partial H}{\partial \mathbf{q}} = 0. \quad (3.32)$$

Rotations

A rotation is defined by a versor $\hat{\mathbf{n}}$ which indicates the axis of rotation and an angle θ . We define $\boldsymbol{\theta} = \theta \hat{\mathbf{n}}$. The angles are taken as positive for anti-clockwise rotations. Let us consider a frame R' rotated by $\boldsymbol{\theta}$ relative to frame R . The component of a vector \mathbf{v} will change according to

$$v'_i = R(\boldsymbol{\theta})_{ij} v_j, \quad (3.33)$$

where $R(\boldsymbol{\theta})$ is the rotation matrix. For infinitesimal transformations

$$\delta \mathbf{v} = \mathbf{v}' - \mathbf{v} \approx -\boldsymbol{\theta} \wedge \mathbf{v}. \quad (3.34)$$

If the quantum system is invariant under rotations it must be possible to construct a unitary transformation on the Hilbert space which realizes the transformation and commutes with the time evolution. Let us then consider the angular momentum

$$\mathbf{J} = \mathbf{q} \wedge \mathbf{p}. \quad (3.35)$$

It is easy to verify that for $\mathbf{v} = \mathbf{q}$ or $\mathbf{v} = \mathbf{p}$ we have

$$[\boldsymbol{\theta} \cdot \mathbf{J}, \mathbf{v}] = -i\boldsymbol{\theta} \wedge \mathbf{v}. \quad (3.36)$$

Then the transformation we are looking for is

$$U(\boldsymbol{\theta}) = e^{i\boldsymbol{\theta} \cdot \mathbf{J}}, \quad (3.37)$$

as can be readily verified for infinitesimal transformations

$$\mathbf{v}' = U^\dagger(\boldsymbol{\theta}) \mathbf{v} U(\boldsymbol{\theta}) \approx \mathbf{v} - i[\boldsymbol{\theta} \cdot \mathbf{J}, \mathbf{v}] = \mathbf{v} - \boldsymbol{\theta} \wedge \mathbf{v}. \quad (3.38)$$

The transformation commutes with the time evolution if

$$[\mathbf{J}, H] = 0 \quad (3.39)$$

which means that H must be a scalar and the angular momentum a constant of motion. Since the transformation is unitary it preserves the commutation relations.

If the particle has a spin the generator of the rotations is the total angular momentum

$$\mathbf{J} = \mathbf{q} \wedge \mathbf{p} + \mathbf{s}. \quad (3.40)$$

Galilean transformations

If we go from a frame R to a frame R' moving relative to R with a constant speed \mathbf{v} we must have

$$\mathbf{q}' = \mathbf{q} - t\mathbf{v}, \quad (3.41)$$

$$\mathbf{p}' = \mathbf{p} - m\mathbf{v}. \quad (3.42)$$

It is easy to verify that these laws of transformation are induced by the unitary operator

$$U(t, \mathbf{v}) = e^{i(\mathbf{p}t - \mathbf{q}m) \cdot \mathbf{v}}, \quad (3.43)$$

so that

$$U^\dagger(t, \mathbf{v})\mathbf{q}U(t, \mathbf{v}) = \mathbf{q} - t\mathbf{v}, \quad (3.44)$$

$$U^\dagger(t, \mathbf{v})\mathbf{p}U(t, \mathbf{v}) = \mathbf{p} - m\mathbf{v}. \quad (3.45)$$

If the Galilean transformation has to be an invariance we must also require

$$U(t, \mathbf{v}) = e^{-iH(t-t')}U(t', \mathbf{v})e^{iH(t-t')}, \quad (3.46)$$

or

$$t\mathbf{p} - m\mathbf{q} = e^{-iH(t-t')}(t'\mathbf{p} - m\mathbf{q})e^{iH(t-t')}. \quad (3.47)$$

If the system is invariant under translations $[\mathbf{p}, H] = 0$, so

$$(t - t')\mathbf{p} = m\mathbf{q} - me^{-iH(t-t')}\mathbf{q}e^{iH(t-t')}. \quad (3.48)$$

For infinitesimal time differences we get

$$\frac{\mathbf{p}}{m} = i[H, \mathbf{q}] = \frac{\partial H}{\partial \mathbf{p}}. \quad (3.49)$$

So

$$H = \frac{\mathbf{p}^2}{2m}. \quad (3.50)$$

Galileo group

We analyzed the symmetries under translations, rotations, and Galileo transformations for a non relativistic system. The corresponding unitary transformations are

$$U(\mathbf{a}) = e^{i\mathbf{a} \cdot \mathbf{p}}, \quad (3.51)$$

$$U(\boldsymbol{\theta}) = e^{i\boldsymbol{\theta} \cdot \mathbf{J}}, \quad (3.52)$$

$$U(\mathbf{v}) = e^{-i\mathbf{v} \cdot \mathbf{K}} \quad \mathbf{K} = m\mathbf{q} - t\mathbf{p} \quad (3.53)$$

The group corresponding to the set of these transformations is called “Galileo group” and the corresponding invariance “galilean invariance”.

From the canonical commutation relationships, the following algebra for the group generators, follows

$$[p_\mu, p_\nu] = 0 \quad P_0 = H \quad (3.54)$$

$$[\mathbf{J}, H] = 0 \quad [J_i, p_j] = i\epsilon_{ijk}p_k \quad (3.55)$$

$$[J_i, J_j] = i\epsilon_{ijk}J_k \quad [J_i, K_j] = i\epsilon_{ijk}K_k \quad (3.56)$$

$$[K_i, K_j] = 0 \quad [K_i, p_j] = im\delta_{ij} \quad [K_i, H] = ip_i \quad (3.57)$$

In the Hilbert space of the physical system is then defined an unitary representation of the group that transforms the spec into itself.

If this representation is reducible it is possible to write the Hilbert space as a direct sum of one or more orthogonal Hilbert spaces each one transforming in itself. The generators are written as sum of the generators acting in each subspace and generators acting on different irreducible subspaces commute. The states in each subspace evolve with their Hamiltonian each in states belonging to the same subspace.

A physical system can then be written as a sum of irreducible representations of the Galileo group.

The simplest case is a particle without internal structure. In this case the only internal variable is the spin which commutes with the orbital variables. A complete set of state is

$$|\mathbf{p}\rangle |s, s_z\rangle. \quad (3.58)$$

Assuming the usual metric

$$\langle \mathbf{p}' | \mathbf{p} \rangle = (2\pi)^3 \delta^3(\mathbf{p} - \mathbf{p}'), \quad (3.59)$$

$$\langle s'_z | s_z \rangle = \delta_{s'_z s_z} \quad (3.60)$$

these states constitute an irreducible representation of the Galileo group if the states $|s_z\rangle$ are an irreducible representation of internal rotations. Let us show this explicitly:

$$\mathbf{p} |\mathbf{p}\rangle = \mathbf{p} |\mathbf{p}\rangle, \quad (3.61)$$

$$\begin{aligned} \mathbf{p} e^{i\boldsymbol{\theta} \cdot \mathbf{J}} |\mathbf{p}\rangle &= e^{i\boldsymbol{\theta} \cdot \mathbf{J}} e^{-i\boldsymbol{\theta} \cdot \mathbf{J}} \mathbf{p} e^{i\boldsymbol{\theta} \cdot \mathbf{J}} |\mathbf{p}\rangle \\ &= R(\boldsymbol{\theta}) \mathbf{p} e^{i\boldsymbol{\theta} \cdot \mathbf{J}} |\mathbf{p}\rangle, \end{aligned} \quad (3.62)$$

where \mathbf{p} on the right hand side denotes the momentum operator acting on the eigenstate $|\mathbf{p}\rangle$ and on the left denotes the eigenvalue. The eigenvalues of the rotated state is the rotated momentum. In the same way:

$$\begin{aligned} \mathbf{p} e^{-i\mathbf{v} \cdot \mathbf{K}} |\mathbf{p}\rangle &= e^{-i\mathbf{v} \cdot \mathbf{K}} e^{i\mathbf{v} \cdot \mathbf{K}} \mathbf{p} e^{-i\mathbf{v} \cdot \mathbf{K}} |\mathbf{p}\rangle \\ &= (\mathbf{p} - m\mathbf{v}) e^{-i\mathbf{v} \cdot \mathbf{K}} |\mathbf{p}\rangle, \end{aligned} \quad (3.63)$$

so

$$e^{i\boldsymbol{\theta} \cdot \mathbf{J}} |\mathbf{p}\rangle = |R(\boldsymbol{\theta})\mathbf{p}\rangle, \quad (3.64)$$

$$e^{-i\mathbf{v} \cdot \mathbf{K}} |\mathbf{p}\rangle = |\mathbf{p} - m\mathbf{v}\rangle, \quad (3.65)$$

and we see that starting from any vector $|\mathbf{p}\rangle$ it is possible to reach any other vector $|\mathbf{p}'\rangle$ through successive applications of rotations or of Galileo transformations. The internal degrees of freedom only transform by rotations independently.

So a pointwise free particle is described by an irreducible unitary representation of the Galileo group.

Parity invariance

The parity transformation is defined by

$$\mathbf{p} \rightarrow -\mathbf{p} \quad \mathbf{q} \rightarrow -\mathbf{q} \quad \mathbf{s} \rightarrow \mathbf{s} \quad (3.66)$$

This is a canonical transformation since it does not change the commutation relations. The transformation operator is

$$U_P = e^{i\frac{\pi}{2}(\mathbf{p} + i\mathbf{q}) \cdot (\mathbf{p} - i\mathbf{q})}. \quad (3.67)$$

The parity transformation has square 1

$$U_P = U_P^{-1} = U_P^\dagger. \quad (3.68)$$

If the parity transformation is an invariance we must have

$$U_P^{-1} H U_P = H \quad (3.69)$$

or

$$[U_P, H] = 0. \quad (3.70)$$

Let us now prove Eq. (3.67) in the one-dimensional case

$$U_P = e^{i\frac{\pi}{2}(p^2 + q^2 - 1)}. \quad (3.71)$$

Apart from a phase this operator coincides with the time evolution operator of a harmonic oscillator of mass 1 and $\omega = 1$ from time $t = 0$ to time $t = \pi$. The Heisenberg equations for

$$q(t) = e^{iHt} q(0) e^{-iHt}, \quad (3.72)$$

$$p(t) = e^{iHt} p(0) e^{-iHt}, \quad (3.73)$$

are

$$\dot{q} = i[H, q], \quad (3.74)$$

$$\dot{p} = i[H, p], \quad (3.75)$$

with $H = (p^2 + q^2)/2$. They have solution

$$q(t) = q \cos t + p \sin t, \quad (3.76)$$

$$p(t) = p \cos t - q \sin t. \quad (3.77)$$

It follows for $t = \pi$

$$q(\pi) = U_P^\dagger q U_P = -q, \quad (3.78)$$

$$p(\pi) = U_P^\dagger p U_P = -p, \quad (3.79)$$

which is what we wanted.

Time reversal

The time reversal acts as follows

$$\mathbf{q} \rightarrow \mathbf{q} \quad \mathbf{p} \rightarrow -\mathbf{p} \quad \mathbf{s} \rightarrow -\mathbf{s} \quad t \rightarrow -t \quad (3.80)$$

This transformation cannot be realized by a unitary operator because in such case the commutation relations would be preserved. Instead we want, in one dimension,

$$[q, p] = i \rightarrow [q, -p] = -i \quad (3.81)$$

If the transformation is antiunitary this is possible:

$$[q', p'] = U_T^\dagger [q, p] U_T = U_T^\dagger i U_T = -i. \quad (3.82)$$

An antilinear operator is defined by

$$T|s_1\rangle = |Ts_1\rangle \quad T|s_2\rangle = |Ts_2\rangle \quad (3.83)$$

$$T(a|s_1\rangle + b|s_2\rangle) = a^* T|s_1\rangle + b^* T|s_2\rangle. \quad (3.84)$$

For a linear operator O

$$\langle a|Ob\rangle = \langle O^\dagger a|b\rangle = \langle b|O^\dagger a\rangle^*, \quad (3.85)$$

and the operator is Hermitian if

$$\langle a|Ob\rangle = \langle Oa|b\rangle. \quad (3.86)$$

For an antilinear operator T

$$\langle a|Tb\rangle = \langle b|T^\dagger a\rangle, \quad (3.87)$$

which is antilinear in $|a\rangle$ and in $|b\rangle$. An antilinear operator is antiunitary if

$$TT^\dagger = T^\dagger T = 1, \quad (3.88)$$

or

$$\langle a|T^\dagger Tb\rangle = \langle Tb|Ta\rangle = \langle a|b\rangle. \quad (3.89)$$

The transformed of O under T

$$O' = T^\dagger O T, \quad (3.90)$$

is still linear and

$$\langle b|T^\dagger O T a\rangle = \langle O T a|T b\rangle = \langle T a|O^\dagger T b\rangle. \quad (3.91)$$

In particular for $O = i$ we find

$$T^\dagger iT = TiT^\dagger = -i. \quad (3.92)$$

The time reversal is realizable with an antiunitary operator:

$$T^\dagger \mathbf{q} T = \mathbf{q} \quad T^\dagger \mathbf{p} T = -\mathbf{p} \quad T^\dagger \mathbf{s} T = -\mathbf{s} \quad (3.93)$$

Moreover, in order to have invariance, we must require

$$T^\dagger H T = H. \quad (3.94)$$

If O is an observable

$$\langle b|OTa\rangle = \langle b|TT^\dagger OTa\rangle = \langle T^\dagger OTa|T^\dagger b\rangle. \quad (3.95)$$

So if $T^\dagger OT = \pm O$ we have

$$\langle b|OTa\rangle = \pm \langle Oa|T^\dagger b\rangle. \quad (3.96)$$

For eigenstates of O , $O|a\rangle = O_a|a\rangle$, we have

$$\langle b|OTa\rangle = \pm O_a \langle a|T^\dagger b\rangle = \pm O_a \langle b|Ta\rangle, \quad (3.97)$$

which means that $|Ta\rangle$ is an eigenstate of O with the transformed eigenvalue.

So for a state $|a\rangle = |\mathbf{p}, s_z\rangle$ we have

$$|Ta\rangle = |-\mathbf{p}, -s_z\rangle, \quad (3.98)$$

modulo a phase.

For a spinless particle with canonical variables \mathbf{q} and \mathbf{p} the time reversal is realized through

$$\langle \mathbf{q}|Ta\rangle = \psi_{Ta}(\mathbf{q}) = \psi_a^*(\mathbf{q}) = \langle \mathbf{q}|a\rangle^*, \quad (3.99)$$

on wave functions in coordinate representation. In fact we have

$$\langle a|T^\dagger \mathbf{p} T b\rangle = \langle \mathbf{p} T b|Ta\rangle = \int \psi_b(\mathbf{q})(-i\nabla)\psi_a^*(\mathbf{q}) d\mathbf{q} = - \int \psi_a^*(\mathbf{q})(-i\nabla)\psi_b(\mathbf{q}) d\mathbf{q} = -\langle a|\mathbf{p} b\rangle, \quad (3.100)$$

where we used an integration by parts. Analogously we verify

$$\langle a|T^\dagger \mathbf{q} T b\rangle = \langle \mathbf{q} T b|Ta\rangle = \langle a|\mathbf{q} b\rangle. \quad (3.101)$$

The Hamiltonian is an Hermitian function of \mathbf{q} and \mathbf{p} . In the coordinate representation, \mathbf{q} is a real variable and $\mathbf{p} = -i\nabla$. The transformation $\mathbf{p} \rightarrow -\mathbf{p}$ is equivalent to a complex conjugation. We will have invariance under T if $H(\mathbf{q}, \mathbf{p}) = H(\mathbf{q}, -\mathbf{p})$ or if H is real. A Hamiltonian of the form

$$H = \frac{\mathbf{p}^2}{2m} + V(\mathbf{q}), \quad (3.102)$$

is invariant under T .

If the particle has spin, it is described by $2s + 1$ functions of \mathbf{q}

$$\psi(\mathbf{q}) = \begin{pmatrix} \psi_1(\mathbf{q}) \\ \vdots \\ \psi_{2s+1}(\mathbf{q}) \end{pmatrix}. \quad (3.103)$$

The spin is represented by three matrices $\mathbf{\Sigma} = (\Sigma_1, \Sigma_2, \Sigma_3)$ independent from \mathbf{q} . We now take

$$\psi_{Ta}(\mathbf{q}) = U\psi_a^*(\mathbf{q}), \quad (3.104)$$

with U an unitary matrix independent from \mathbf{q} and acting on spin space. To have the correct spin transformations we must have

$$\langle a|T^\dagger \mathbf{s} T b\rangle = \langle \mathbf{s} T b|Ta\rangle = -\langle a|\mathbf{s} b\rangle, \quad (3.105)$$

or

$$-\int \psi_a^\dagger \mathbf{\Sigma} \psi_b = \int \psi_b^{\text{Tr}} U^\dagger \mathbf{\Sigma} U \psi_a^*, \quad (3.106)$$

which means

$$U^{\text{Tr}} \mathbf{\Sigma}^{\text{Tr}} U^{\dagger \text{Tr}} = -\mathbf{\Sigma}, \quad (3.107)$$

and taking the complex conjugate, since $\mathbf{\Sigma}^\dagger = \mathbf{\Sigma}$, we find

$$U^\dagger \mathbf{\Sigma} U = -\mathbf{\Sigma}^*. \quad (3.108)$$

With the usual choice of phases in the angular momentum representation Σ_1 and Σ_3 are real matrices and Σ_2 is pure imaginary.

For example for spin 1/2 particles

$$\Sigma_3 = \frac{1}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad \Sigma_1 = \frac{1}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \Sigma_2 = \frac{1}{2} \begin{pmatrix} 0 & i \\ -i & 0 \end{pmatrix} \quad (3.109)$$

Then apart from an unessential phase we find

$$U = e^{i\pi \Sigma_2}, \quad (3.110)$$

a rotation of π around the 2 axis, which changes sign to Σ_1 and Σ_3 . In conclusions we have

$$\psi_{Ta} = e^{i\pi \Sigma_2} \psi_a^*. \quad (3.111)$$

C. Einstein Relativity

The invariance under the Galileo group is valid in the limit of small velocities. But, actually, physics is invariant under Lorentz transformations in addition to spatial translations. This invariance is known as Einstein relativity.

The Lorentz group is defined as the group of linear transformations which leaves invariant the quadratic form

$$ds^2 = dt^2 - d\mathbf{x}^2. \quad (3.112)$$

Let $dx = (dx^0, dx^1, dx^2, dx^3) = (dt, d\mathbf{x})$ we can write

$$ds^2 = g_{\mu\nu} dx^\mu dx^\nu, \quad (3.113)$$

where Einstein summation convention is used with

$$g_{\mu\nu} = g^{\mu\nu} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} \quad g^{\mu\nu} g_{\nu\alpha} = \delta^\mu_\alpha \quad (3.114)$$

The Lorentz transformations are defined as the linear transformations

$$dx'^\mu = \Lambda^\mu_\nu dx^\nu, \quad (3.115)$$

such that

$$g_{\mu\nu} dx'^\mu dx'^\nu = g_{\mu\nu} \Lambda^\mu_\alpha \Lambda^\nu_\beta dx^\alpha dx^\beta. \quad (3.116)$$

Due to the arbitrariness of dx^μ we have

$$g_{\mu\nu} = g_{\alpha\beta} \Lambda^\alpha_\mu \Lambda^\beta_\nu, \quad (3.117)$$

or

$$\mathbf{g} = \mathbf{\Lambda}^{\text{Tr}} \mathbf{g} \mathbf{\Lambda}, \quad (3.118)$$

which defines the Lorentz group. Taking the 00 component in Eq. (3.117)

$$1 = g_{\alpha\beta} \Lambda^\alpha_0 \Lambda^\beta_0 = (\Lambda^0_0)^2 - \sum_i (\Lambda^i_0)^2, \quad (3.119)$$

or

$$(\Lambda_0^0)^2 \geq 1, \quad (3.120)$$

or

$$\Lambda_0^0 \geq 1 \quad \text{or} \quad \Lambda_0^0 \leq -1. \quad (3.121)$$

Taking the determinant in Eq. (3.117) follows

$$(\det \mathbf{\Lambda})^2 = 1, \quad (3.122)$$

or

$$\det \mathbf{\Lambda} = \pm 1. \quad (3.123)$$

The transformations obtained continuously from the identity have $\Lambda_0^0 \geq 1$ and $\det \mathbf{\Lambda} = 1$ and constitute the *proper* Lorentz group. The transformations with $\Lambda_0^0 \geq 1$ and $\det \mathbf{\Lambda} = -1$ can be written as the product of the parity $P : \mathbf{x} \rightarrow -\mathbf{x}$ times a proper transformation. The ones with $\Lambda_0^0 \leq -1$ and $\det \mathbf{\Lambda} = 1$ as a product of the time reversal $T : x^0 \rightarrow -x^0$ times the proper transformations. The ones with $\Lambda_0^0 \leq -1$ and $\det \mathbf{\Lambda} = -1$ as PT times a proper transformation.

An infinitesimal proper transformation

$$\Lambda_{\mu'}^{\mu} = \delta_{\mu'}^{\mu} + \Omega_{\mu'}^{\mu}, \quad (3.124)$$

must satisfy Eq. (3.117). So

$$g_{\mu'\nu'} = g_{\mu\nu} + \Omega_{\mu'}^{\mu} g_{\mu\nu} + \Omega_{\nu'}^{\nu} g_{\mu\nu} + \mathcal{O}(\Omega^2). \quad (3.125)$$

Let

$$\Omega_{\mu\nu} = g_{\mu\alpha} \Omega_{\nu}^{\alpha}, \quad (3.126)$$

then we must have

$$\Omega_{\mu\nu} = -\Omega_{\nu\mu}. \quad (3.127)$$

The group has 6 parameters as the number of components of an antisymmetric 4×4 matrix. The most general 4×4 antisymmetric matrix can be written as

$$\Omega_{\mu\nu} = \frac{1}{2} \sum_{\rho\sigma} \omega_{(\rho\sigma)} M_{\mu\nu}^{(\rho\sigma)}, \quad (3.128)$$

$$M_{\mu\nu}^{(\rho\sigma)} = \delta_{\mu}^{\rho} \delta_{\nu}^{\sigma} - \delta_{\nu}^{\rho} \delta_{\mu}^{\sigma} = -M_{\mu\nu}^{(\sigma\rho)}. \quad (3.129)$$

We write

$$\left(M^{(\rho\sigma)} \right)_{\nu}^{\mu} = g^{\mu\alpha} M_{\alpha\nu}^{(\rho\sigma)}, \quad (3.130)$$

so

$$\Omega_{\nu}^{\mu} = g^{\mu\alpha} \Omega_{\alpha\nu} = g^{\mu\alpha} \frac{1}{2} \omega_{(\rho\sigma)} M_{\alpha\nu}^{(\rho\sigma)} = \frac{1}{2} \omega_{(\rho\sigma)} \left(M^{(\rho\sigma)} \right)_{\nu}^{\mu}. \quad (3.131)$$

The matrices $M^{(\mu\nu)}$ satisfy the following algebra

$$[M^{(\alpha\beta)}, M^{(\mu\nu)}] = - \left(g^{\alpha\mu} M^{(\beta\nu)} + g^{\beta\nu} M^{(\alpha\mu)} - g^{\beta\mu} M^{(\alpha\nu)} - g^{\alpha\nu} M^{(\beta\mu)} \right). \quad (3.132)$$

We can then introduce

$$J^{(\mu\nu)} \equiv -i M^{(\mu\nu)}, \quad (3.133)$$

and

$$J^i = -\frac{1}{2} \epsilon_{0ijk} J^{(jk)}, \quad (3.134)$$

$$K^i = J^{(0i)}, \quad (3.135)$$

where $\epsilon_{\mu_0\mu_1\mu_2\mu_3}$ is the Levi-Civita symbol with $\epsilon_{0123} = 1$ ⁷. Then Eq. (3.132) is rewritten as

$$[J^i, J^j] = i\epsilon_{ijk}J^k, \quad (3.139)$$

$$[J^i, K^j] = i\epsilon_{ijk}K^k, \quad (3.140)$$

$$[K^i, K^j] = -i\epsilon_{ijk}J^k. \quad (3.141)$$

The generators J^i are the rotations generators, which constitute a subgroup of the Lorentz transformations. The K^i are the generators of the velocity (\mathbf{v}) transformations and are vectors, as follows from their commutation relations with the J^i . The infinitesimal transformations are then

$$\mathbf{\Lambda} = 1 + i(\boldsymbol{\theta} \cdot \mathbf{J} - \boldsymbol{\alpha} \cdot \mathbf{K}). \quad (3.142)$$

The finite ones are

$$\mathbf{\Lambda} = e^{\frac{i}{2} \sum_{\alpha\beta} J^{(\alpha\beta)} \omega_{(\alpha\beta)}} = e^{i(\boldsymbol{\theta} \cdot \mathbf{J} - \boldsymbol{\alpha} \cdot \mathbf{K})} \quad \mathbf{v} = (\tanh \alpha_1, \tanh \alpha_2, \tanh \alpha_3), \quad (3.143)$$

where $\boldsymbol{\theta}$ is the rotation angle vector and $\boldsymbol{\alpha}$ is the rapidity vector.

Under the Lorentz group the generators of the translations p_μ must transform as four-vectors

$$[J^{(\mu\nu)}, p^\alpha] = i(g^{\mu\alpha}p^\nu - g^{\alpha\nu}p^\mu), \quad (3.144)$$

or

$$[\mathbf{J}, p^0] = -\delta p^0 = -\mathbf{J}p^0 = 0, \quad (3.145)$$

which expresses the conservation of angular momentum, and

$$[J^i, p^j] = -\delta p^j = -J^i p^j = i\epsilon_{ijk}p^k, \quad (3.146)$$

which tells us that \mathbf{p} is a vector. On the momenta the generators of the velocity transformations act as follows

$$[K^i, p^0] = -\delta p^0 = -K^i p^0 = ig^{00}p^i, \quad (3.147)$$

$$[K^i, p^j] = -\delta p^j = -K^i p^j = -ig^{ij}p^0. \quad (3.148)$$

The invariance under translations is written as

$$[p^\mu, p^\nu] = 0. \quad (3.149)$$

The commutation relations between the generators are then

$$[p^\mu, p^\nu] = 0, \quad (3.150)$$

$$[J^{(\mu\nu)}, p^\alpha] = i(g^{\mu\alpha}p^\nu - g^{\alpha\nu}p^\mu), \quad (3.151)$$

$$[J^{(\alpha\beta)}, J^{(\mu\nu)}] = i(g^{\alpha\mu}J^{(\beta\nu)} + g^{\beta\nu}J^{(\alpha\mu)} - g^{\beta\mu}J^{(\alpha\nu)} - g^{\alpha\nu}J^{(\beta\mu)}). \quad (3.152)$$

They define the Lie algebra of a 10 parameters group known as the Poincaré group.

The Poincaré group is defined by the transformation laws

$$(\Lambda, a) : x \rightarrow x' = \mathbf{\Lambda}x - a, \quad (3.153)$$

where a is a translation and Λ is a Lorentz transformation. We immediately find the multiplication properties of the group as

$$(\Lambda_1, a)(\Lambda_2, b) = (\Lambda_1\Lambda_2, -\Lambda_1b - a), \quad (3.154)$$

from which immediately follows that the translations are an abelian invariant subgroup. In fact applying repetitively Eq. (3.154) we find that the transformed by similitude of a translation $(1, a)$,

$$(\Lambda, c)(1, a)(\Lambda^{-1}, -c) = (1, \Lambda(c - a) - c), \quad (3.155)$$

⁷ For any antisymmetric tensor $F^{\mu\nu}$ it is possible to use a decomposition of the following kind: $F^{\mu\nu} = (\mathbf{P}, \mathbf{A})$ with

$$A^1 = -F^{23} \quad A^2 = -F^{31} \quad A^3 = -F^{12} \quad (3.136)$$

$$P^1 = F^{01} \quad P^2 = F^{02} \quad P^3 = F^{03} \quad (3.137)$$

For the product of two tensors of this kind we have

$$\frac{1}{2}F_{\mu\nu}^{(1)}F^{(2)\mu\nu} = \mathbf{A}^{(1)} \cdot \mathbf{A}^{(2)} - \mathbf{P}^{(1)} \cdot \mathbf{P}^{(2)}. \quad (3.138)$$

is still a translation.

By Wigner theorem the states of a physical system are the basis of a unitary representation of the Poincaré group. An elementary system will be described by an irreducible representation of the Poincaré group.

We note that

$$\mathbf{J}_\pm = \frac{\mathbf{J} \pm i\mathbf{K}}{2}, \quad (3.156)$$

obey the following commutation relations

$$[J_+^i, J_+^j] = i\epsilon_{ijk}J_+^k, \quad (3.157)$$

$$[J_-^i, J_-^j] = i\epsilon_{ijk}J_-^k, \quad (3.158)$$

$$[J_+^i, J_-^j] = 0. \quad (3.159)$$

So the generators of \mathbf{J}_+ and \mathbf{J}_- obey to the algebra $SU(2) \otimes SU(2)$. Let us show now that an irreducible representation of the Poincaré group, i.e. an elementary particle, is determined by the mass and the spin.

An irreducible representation is characterized by the value of the *invariants*, i.e. of the operators built with the generators of the group that commute with all the group generators. We then define

$$\Gamma_\mu = \frac{1}{2}\epsilon_{\mu\alpha\beta\sigma}J^{(\alpha\beta)}p^\sigma, \quad (3.160)$$

$$\Gamma_\mu p^\mu = 0, \quad (3.161)$$

$$g^\mu = J^{(\mu\nu)}p_\nu, \quad (3.162)$$

$$g^\mu p_\mu = 0. \quad (3.163)$$

One can prove [16–18]⁸ that

$$p^2 J^{(\mu\nu)} = g^\mu p^\nu - g^\nu p^\mu - \epsilon^{\sigma\mu\nu\lambda}\Gamma_\sigma p_\lambda. \quad (3.165)$$

This tells us that $J^{(\mu\nu)}$ can be expressed in terms of p_μ, Γ_μ , and g_μ if $p^2 = p_\mu p^\mu \neq 0$.

Moreover we have

$$[\Gamma_\mu, \Gamma_\nu] = i\epsilon_{\rho\mu\nu\lambda}\Gamma^\rho p^\lambda, \quad (3.166)$$

$$[g_\mu, \Gamma_\sigma] = -i\Gamma_\mu p_\sigma, \quad (3.167)$$

$$[g_\mu, p_\nu] = i(g_{\mu\nu}p^2 - p_\mu p_\nu), \quad (3.168)$$

$$[g_\mu, g_\nu] = -i(g^\mu p^\nu - g^\nu p^\mu - \epsilon^{\sigma\mu\nu\lambda}\Gamma_\sigma p_\lambda) \quad (3.169)$$

$$[p_\mu, \Gamma_\sigma] = 0. \quad (3.170)$$

An invariant should be constructed with the vectors p_μ, Γ_μ , and g_μ . Recalling that $g_\mu p^\mu = 0$ and $\Gamma_\mu p^\mu = 0$ the only independent invariants under the Lorentz group are

$$p^2, \Gamma^2, g^2, \Gamma_\mu g^\mu. \quad (3.171)$$

But g^2 and $\Gamma_\mu g^\mu$ do not commute with translations. Then the representation is determined by p^2, Γ^2 , and by the sign of p^0 , which is also invariant under the proper Lorentz group and commutes with translations, if $p^2 \geq 0$.

The physical interpretation of the two invariants is obvious:

i. For the invariant p^2 we have 4 cases

$$p^2 > 0, \quad (3.172)$$

$$p^2 = 0 \quad p \neq 0, \quad (3.173)$$

$$p^2 = 0 \quad p = 0, \quad (3.174)$$

$$p^2 < 0. \quad (3.175)$$

Since $p^2 = m^2$ we will be interested only in the first two cases. In these two cases, for the representations of the proper group ($\Lambda^0_0 \geq 0$ and $\det \Lambda = 1$) we will have another invariant, namely the sign of p^0 .

⁸ One can use the identity

$$\epsilon^{\sigma\mu\nu\lambda}\epsilon_{\sigma\alpha\beta\rho} = \det \begin{pmatrix} \delta^\mu_\alpha & \delta^\mu_\beta & \delta^\mu_\rho \\ \delta^\nu_\alpha & \delta^\nu_\beta & \delta^\nu_\rho \\ \delta^\lambda_\alpha & \delta^\lambda_\beta & \delta^\lambda_\rho \end{pmatrix}, \quad (3.164)$$

and the definition of Γ_σ to calculate the product $\epsilon^{\sigma\mu\nu\lambda}\Gamma_\sigma p_\lambda$.

ii. The invariant Γ^2 can be calculated in the reference frame where $\mathbf{p} = 0$. In such a frame

$$\Gamma = (\Gamma^0, \Gamma^1, \Gamma^2, \Gamma^3) = (\Gamma^0, \mathbf{\Gamma}) = (0, m\mathbf{J}) \quad \Gamma^2 = -m^2 J(J+1). \quad (3.176)$$

The modulus of \mathbf{J} in the rest frame is by definition the particle spin, so $\Gamma^2 = -m^2 s(s+1)$

Then the representation is determined by the mass m and by the spin s , exactly as in the nonrelativistic happens for the Galileo group.

IV. IN CLASSICAL FIELD THEORY [6]

In this section we will work in Minkowski spacetime $x = (x^0, x^1, x^2, x^3) = (t, \mathbf{x})$ with the metric (3.114) $g_{\mu\nu} = \eta_{\mu\nu} = \text{diag}(1, -1, -1, -1)$. We will denote with $\partial_\mu = \partial/\partial x^\mu$ and adopt Einstein convention to subtend a sum over repeated indexes. We will use greek indexes for all 4 spacetime components and roman indexes for only the 3 spatial components.

Theorem IV.1. *If the action is invariant under a local transformation $x \rightarrow x'$, $\varphi(x) \rightarrow \varphi'(x') = T\varphi(x)$ in the sense that, for any domain D and the corresponding transformed domain D'*

$$S_D = \int_D \mathcal{L}[\varphi(x), \partial_\mu \varphi(x)] d^4x = S_{D'} = \int_{D'} \mathcal{L}[\varphi'(x'), \partial'_\mu \varphi'(x')] d^4x', \quad (4.1)$$

where the Lagrangian \mathcal{L} is the same function of the initial fields and of the transformed fields, then the equations of motion are invariant in form under the transformation, i.e. on the two reference frames one experiences the same physics.

Proof. An arbitrary variation $\delta\varphi(x)$ vanishing on the frontier of domain D produces a variation $\delta\varphi'(x') = T\delta\varphi(x)$ vanishing on the frontier of D' (see Fig. 4). Since we identically have $S_D = S_{D'}$, the stationary principle $\delta S_D = 0$ implies $\delta S_{D'} = 0$ and the resulting equations of motion for $\varphi(x)$ and $\varphi'(x')$ have the same form. \square

If additionally to the Lagrangian form invariance

$$\mathcal{L}[\varphi(x), \partial_\mu \varphi(x)] = \mathcal{L}[\varphi'(x'), \partial'_\mu \varphi'(x')], \quad (4.2)$$

we also have that the Jacobian of the transformation $J(x, x') = 1$ then $S_D = S_{D'}$ and we will have invariance under the local transformation.

A Lagrangian that transforms as a scalar density under the Poincaré group (3.153), parity (3.66), and time reversal (3.80) will then be invariant under these transformations, since their Jacobian is 1.

A. Noether theorem

Amalie Emmy Noether (Erlangen, 23 March 1882 – Bryn Mawr, 14 April 1935) formulated the following theorem:

Theorem IV.2 (Noether). *If S_D is an invariant action under a group of continuous transformations and*

$$x^\mu \rightarrow x'^\mu = x^\mu + \delta x^\mu \quad \text{with} \quad \delta x^\mu = A_a^\mu \delta\omega^a \quad (4.3)$$

$$\varphi_i \rightarrow \varphi'_i(x') = (\delta_{ij} + M_{ij}^a \delta\omega^a) \varphi_j(x), \quad (4.4)$$

are the infinitesimal transformations of parameters $\delta\omega^a$, then the currents

$$J_a^\mu = \frac{\partial \mathcal{L}}{\partial(\partial_\mu \varphi_i)} [A_a^\nu \partial_\nu \varphi_i(x) - M_{ij}^a \varphi_j(x)] - A_a^\mu \mathcal{L}, \quad (4.5)$$

are conserved, in the sense that

$$\partial_\mu J_a^\mu(x) = 0. \quad (4.6)$$

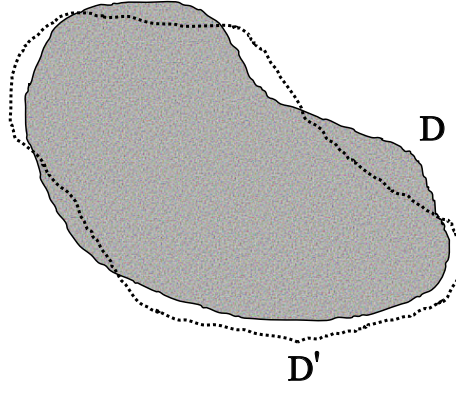


FIG. 4. Domains of integration in the initial action and its transformed.

Proof. The invariance under the infinitesimal transformation implies

$$\int_{D'} \mathcal{L}[\varphi'(x'), \partial'_\mu \varphi'(x')] d^4 x' = \int_D \mathcal{L}[\varphi(x), \partial_\mu \varphi(x)] d^4 x, \quad (4.7)$$

where the domains of integration are shown in Fig. 4. We may also write

$$\int_{D'} \mathcal{L}[\varphi'(x'), \partial'_\mu \varphi'(x')] d^4 x' \approx \int_D \mathcal{L}[\varphi'(x), \partial_\mu \varphi'(x)] d^4 x + \int_{\partial D} \mathcal{L}[\varphi(x), \partial_\mu \varphi(x)] \delta x^\alpha d^3 \Sigma_\alpha, \quad (4.8)$$

where in the second integral in the right hand side φ' has been approximated with φ since the deformations δx^α are already infinitesimal of the first order and we want to neglect infinitesimals of higher order than the first.

On the other hand $\varphi'(x') = (1 + M_a \delta \omega^a) \varphi(x)$ and neglecting terms of second order⁹

$$\begin{aligned} \varphi'(x) &\approx (1 + M_a \delta \omega^a) \varphi(x) - \delta x^\mu \partial_\mu \varphi(x) \\ &= \varphi(x) + [M_a \varphi(x) - A_a^\mu \partial_\mu \varphi(x)] \delta \omega^a = \varphi(x) + \bar{\delta} \varphi(x). \end{aligned} \quad (4.9)$$

Starting from (4.8) and using Gauss theorem

$$0 = S_D - S_{D'} = \int_D \left[-\frac{\partial \mathcal{L}}{\partial \varphi_i} \bar{\delta} \varphi_i - \frac{\partial \mathcal{L}}{\partial (\partial_\mu \varphi_i)} \partial_\mu \bar{\delta} \varphi_i - \partial_\mu (\mathcal{L} \delta x^\mu) \right] d^4 x. \quad (4.10)$$

Using the equations of motion

$$\frac{\partial \mathcal{L}}{\partial \varphi_i} = \partial_\mu \frac{\partial \mathcal{L}}{\partial (\partial_\mu \varphi_i)}, \quad (4.11)$$

we find

$$\begin{aligned} 0 &= \int_D \partial_\mu \left[-\frac{\partial \mathcal{L}}{\partial (\partial_\mu \varphi_i)} \bar{\delta} \varphi_i - \mathcal{L} \delta x^\mu \right] d^4 x \\ &= \delta \omega^a \int_D \partial_\mu \left[\frac{\partial \mathcal{L}}{\partial (\partial_\mu \varphi_i)} (A_a^\nu \partial_\nu \varphi_i - M_{ij}^a \varphi_j) - A_a^\mu \mathcal{L} \right] d^4 x, \end{aligned} \quad (4.12)$$

from which follows the thesis (4.6) from the arbitrariness of D and $\delta \omega^a$. \square

Lemma IV.3. *An immediate consequence of Theorem IV.2 is that the charge*

$$Q_a(t) = \int J_a^0(t, \mathbf{x}) d^3 \mathbf{x}, \quad (4.13)$$

is independent of time

$$\frac{dQ_a(t)}{dt} = 0. \quad (4.14)$$

⁹ Note that $\varphi'(x') = \varphi'(x + \delta x) \approx \varphi'(x) + \delta x^\mu \partial_\mu \varphi'(x) = \varphi'(x) + \delta x^\mu \partial_\mu \varphi(x)$ where in the first equality we expanded in a Taylor series truncated to first order and in the second equality we replaced $\varphi'(x)$ with $\varphi(x)$ since we neglect terms of order higher than the first.

Proof. To prove Lemma IV.3 we note that from Eq. (4.6) follows

$$\frac{dQ_a(t)}{dt} = - \int_{\Omega} \partial_k J^k(x) d^3 \mathbf{x} = - \int_{\partial\Omega} J^k d^2 S_k = 0 \quad (4.15)$$

where in the second equation we used Gauss theorem and in the last equality we note that since there are no sources of current within the domain Ω the current flux through the surface enclosing the domain $\partial\Omega$ must be zero. \square

B. Conserved quantities

Let us now consider some examples of invariance that give rise to conserved currents and to their corresponding conserved quantities. The first two examples refer to spacetime transformations, i.e. the translations and the Lorentz transformations that give rise, as conserved quantities, to the energy-momentum tensor and to the density of angular momentum. The other two examples refer to “internal” symmetries.

Translational invariance

For translations

$$\delta\omega^\nu = a^\nu, \quad M_{ij}^a = 0, \quad A_a^\nu = \delta_a^\nu. \quad (4.16)$$

If there is invariance the conserved quantity is

$$Q^{\mu\nu} = \frac{\partial \mathcal{L}}{\partial(\partial_\mu \varphi_i)} \partial^\nu \varphi_i - \mathcal{L} g^{\mu\nu}, \quad (4.17)$$

that is the energy-momentum tensor. The conserved 4-momentum is

$$P^\nu = \int Q^{0\nu}(t, \mathbf{x}) d^3 \mathbf{x} = \int \left[\frac{\partial \mathcal{L}}{\partial(\partial_0 \varphi_i)} \partial^\nu \varphi_i - \mathcal{L} g^{0\nu} \right] d^3 \mathbf{x}. \quad (4.18)$$

For a free scalar field

$$\mathcal{L} = \frac{1}{2}(\partial_\alpha \varphi \partial^\alpha \varphi - m^2 \varphi^2), \quad (4.19)$$

we have

$$Q_{\mu\nu} = \partial_\mu \varphi \partial_\nu \varphi - \frac{1}{2}(\partial_\alpha \varphi \partial^\alpha \varphi - m^2 \varphi^2) \quad (4.20)$$

Lorentz transformations invariance

Under a Lorentz transformation

$$\delta x^\mu = \omega^{\mu\alpha} x_\alpha = \frac{1}{2}(\delta^\mu_\rho \delta^\nu_\sigma - \delta^\mu_\sigma \delta^\nu_\rho) x_\nu \omega^{\rho\sigma}. \quad (4.21)$$

The conserved quantity is the angular momentum tensor

$$S^{\mu,\nu\tau} = x^\tau Q^{\mu\nu} - x^\nu Q^{\mu\tau} - \frac{\partial \mathcal{L}}{\partial(\partial_\mu \varphi_i)} M_{ij}^{\nu\tau} \varphi_j, \quad (4.22)$$

where $Q^{\mu\nu}$ is the energy-momentum tensor of Eq. (4.17).

For a scalar field $M_{ij}^{\nu\tau} = 0$ and

$$S^{\mu,\nu\tau} = x^\tau Q^{\mu\nu} - x^\nu Q^{\mu\tau}. \quad (4.23)$$

The conservation of the energy-momentum tensor

$$\partial_\mu Q^{\mu\nu} = 0, \quad (4.24)$$

together with the Lorentz invariance implies

$$0 = \partial_\mu S^{\mu,\nu\tau} = Q^{\tau\nu} - Q^{\nu\tau}, \quad (4.25)$$

i.e. the energy-momentum tensor is symmetric. The constants of motion associated to the Lorentz invariance are

$$\int [x^\tau Q^{0\nu} - x^\nu Q^{0\tau}] d^3\mathbf{x}. \quad (4.26)$$

For τ, ν spatial, these represent the density of orbital angular momentum of the system. For $\tau = 0$ and $\nu = i$ they impose that

$$p^i = \frac{d}{dt} \int Q^{00} x^i d^3\mathbf{x}, \quad (4.27)$$

where

$$p^i = \int Q^{0i} d^3\mathbf{x}, \quad (4.28)$$

is the conserved total momentum. Eq. (4.27) tells that the center of mass of the system undergoes uniform rectilinear motion.

U(1) transformations

If the action is invariant under the transformation

$$\varphi_i(x) \rightarrow e^{-i\alpha q_i} \varphi_i(x), \quad \delta\varphi_i = -i\alpha q_i \varphi_i, \quad (4.29)$$

parametrized by the phase α , with q_i a number that depends on the kind of field i , $A_a^\mu = 0$ and $M_{ij}^a = -iq_i \delta_{ij}$, the current is

$$J_\mu = i \frac{\partial \mathcal{L}}{\partial(\partial^\mu \varphi_i)} q_i \varphi_i, \quad (4.30)$$

and the corresponding charge

$$Q = \int J^0(t, \mathbf{x}) d^3\mathbf{x}. \quad (4.31)$$

For example for a (complex) scalar field

$$\varphi \rightarrow \varphi e^{ie\alpha}, \quad \varphi^* \rightarrow \varphi^* e^{-ie\alpha}, \quad (4.32)$$

with charges $\pm e$.

Transformations under groups of internal symmetry

If the action is invariant under a group of internal symmetry

$$\delta x^\mu = 0, \quad \varphi \rightarrow e^{iT^a \omega^a} \varphi, \quad (4.33)$$

where T^a are the generators of the group, then the conserved currents are

$$J_\mu^a = -i \frac{\partial \mathcal{L}}{\partial(\partial^\mu \varphi)} T^a \varphi. \quad (4.34)$$

V. IN GENERAL RELATIVITY [7]

Spacetime is described by a pseudo Riemannian manifold of dimension 4 with a metric tensor $g_{\mu\nu}$ on which we have a system of coordinates $\vec{x} = (x^0, x^1, x^2, x^3) = (t, \mathbf{x})$.

An *isometry* is a transformation that leaves the metric tensor unchanged. We will deal with continuous transformations.

A. Killing vectors

Consider a vector field $\vec{\xi}$ and choose spacetime coordinates such that $\vec{\xi} = \partial/\partial t$. $\vec{\xi}$ is a *killing vector* if $\partial g_{\mu\nu}/\partial t = g_{\mu\nu,0} = 0$, where as usual we indicate with a comma a partial derivative.

We will now prove that $\vec{\xi}$ is a killing vector if and only if

$$\xi_{\mu;\nu} + \xi_{\nu;\mu} = 0, \quad (5.1)$$

where as usual we indicate with a semicolon the covariant derivative. Eq. (5.1) is known as the *killing equation* and this property of ξ is the coordinate characterization of the killing vector.

Consider then

$$\xi_{\mu;\nu} = g_{\mu\alpha} \xi^\alpha_{;\nu} = g_{\mu\alpha} (\xi^\alpha_{;\nu} + \Gamma^\alpha_{\beta\nu} \xi^\beta) = \Gamma_{\mu 0\nu} = \frac{1}{2} (g_{\mu 0,\nu} + g_{\mu\nu,0} - g_{0\nu,\mu}), \quad (5.2)$$

where as usual we use Einstein convention of tacitly assuming a summation over repeated indexes, in the first equality we used the covariant invariance of the metric tensor, in the second equation we used the definition of the covariant derivative, where we denoted with Γ the Christoffel symbol, in the third equation we used the fact that $\xi^\alpha = \delta^\alpha_0$, and in the last equality we used the definition of the Christoffel symbol. Using then the fact that the metric tensor is symmetric we find $\xi_{\mu;\nu} + \xi_{\nu;\mu} = g_{\mu\nu,0} = 0$. This proves the killing equation (5.1).

The killing vectors have the following 3 properties. If $\vec{\xi}$ and \vec{p} are killing vectors then:

- i. $[\vec{\xi}, \vec{p}] = \vec{\xi} \cdot \vec{p} - \vec{p} \cdot \vec{\xi}$ is a killing vector;
- ii. $a\vec{\xi} + b\vec{p}$, with a, b constants, is a killing vector;
- iii. if \vec{p} is the 4-momentum of a free particle of rest mass m then $\vec{p} \cdot \vec{\xi}$ is a constant of motion.

The first two properties are proven in Exercise 10.3 of [19]. We are here interested in the third property

$$\nabla_{\vec{p}}(\vec{p} \cdot \vec{\xi}) = (\nabla_{\vec{p}}\vec{p}) \cdot \vec{\xi} + \vec{p} \cdot (\nabla_{\vec{p}}\vec{\xi}) = \vec{p} \cdot (\nabla_{\vec{p}}\vec{\xi}) = p^\mu p^\nu \xi_{\mu;\nu} = 0, \quad (5.3)$$

where in the second equality we used the fact that the particle parallel transports herself along her worldline, $\nabla_{\vec{p}}\vec{p} = 0$, and in the last equality we used the killing equation (5.1). This third property then tells us that $\vec{p} \cdot \vec{\xi}$ is constant along the particle world line since $D/d\tau = \vec{p} \cdot \nabla_{\vec{p}}$, with τ the particle proper time, is a covariant derivative.

Moreover, at an event \mathcal{P} of spacetime, we may write $\vec{p} \cdot \vec{\xi} = m \lim_{\tau \rightarrow 0} [\vec{x}'(\mathcal{P}) - \vec{x}(\mathcal{P})] \cdot \vec{\xi} / \tau = q$ with q a constant. Then, for an infinitesimal proper time τ , we have

$$\vec{x}'(\mathcal{P}) \approx \vec{x}(\mathcal{P}) + \epsilon \vec{\xi}, \quad (5.4)$$

with $\epsilon = \tau q / (m \xi^\mu \xi_\mu)$.

In flat spacetime

Choose an inertial Local Lorentz Frame (LLF) at an event \mathcal{P} of spacetime so that $g_{\mu\nu} = \eta_{\mu\nu}$ with $\|\eta_{\mu\nu}\| = \text{diag}(1, -1, -1, -1)$ Minkowski metric. Then the Christoffel symbols Γ vanish and the killing equation simply becomes

$$\xi_{\mu,\nu} + \xi_{\nu,\mu} = 0, \quad (5.5)$$

from which follows that there are only 10 independent constraints whose solutions can be found as follows:

- i There will be 4

$$\xi^\mu(\alpha) = a^\mu(\alpha), \quad \alpha = 0, 1, 2, 3. \quad (5.6)$$

These represents 4-translations. For example, we may choose the 4 constant vectors as $a^\mu(\alpha) = \delta^\mu_\alpha$, pointing in each of the 4 directions of the frame. For example, for $a^\mu(1) = \delta^\mu_1$, $\vec{\xi}(1) = \partial/\partial x$ and (5.4) represents a translation along the x direction, $x' \approx x + \epsilon$.

ii There will be 6

$$\xi^\mu(\alpha) = \omega^{\mu\nu}(\alpha)x^\nu, \quad (5.7)$$

where $\omega^{\mu\nu}$ are antisymmetric constants. In fact

$$\xi^\mu_{,\alpha} + \xi^\alpha_{,\mu} = \omega^{\mu\nu}x^\nu_{,\alpha} + \omega^{\alpha\nu}x^\nu_{,\mu} = \omega^{\mu\alpha} + \omega^{\alpha\mu} = 0, \quad (5.8)$$

so the choice (5.7) satisfies the killing equation. We will now show how the infinitesimal coordinate transformations induced by the $\vec{\xi}$ of (5.7) constitute the *Lorentz group*: 3 rotations and 3 boosts:

i. The 3 rotations are generated by the choice

$$\xi^0(k) = 0, \quad \xi^i(k) = \epsilon^{ikm}x^m, \quad k = 1, 2, 3, \quad (5.9)$$

where as usual we use roman indexes to denote the spatial components. So, for example, $\vec{\xi}(1) = y\partial/\partial z - z\partial/\partial y$ represents a rotation (5.4) around the x axis of an infinitesimal angle ϵ .

ii. The 3 boosts are generated by choosing

$$\xi^\mu(k) = 2g^{\mu\nu}\delta_\nu^{[0}x^{k]}, \quad k = 1, 2, 3, \quad (5.10)$$

where the square parenthesis around two indexes denotes their antisymmetrization. So, for example, $\vec{\xi}(1) = x\partial/\partial t + t\partial/\partial x$ represents a boost (5.4) along the x direction of infinitesimal velocity $\beta = \epsilon$ for which $\gamma = 1/\sqrt{1-\beta^2} \approx 1$.

So the killing vectors of flat spacetime induce the infinitesimal coordinate transformations of the *Poincaré group* (the inhomogeneous Lorentz group).

In the global spacetime there are in general no killing vectors.

In correspondence of the 10 killing vectors there are 10 currents and then 10 conserved scalar quantities.

Conserved quantities in Minkowski spacetime

Given the stress-energy tensor $T_{\mu\nu}$, we may define the following *currents*

$$J^\mu(\alpha) = T^{\mu\nu}\xi_\nu(\alpha), \quad \alpha = 1, 2, 3, \dots, 10, \quad (5.11)$$

such that

$$J^\mu_{,\mu} = T^{\mu\nu}\xi_{\nu,\mu} = 0, \quad (5.12)$$

where in the first equality we used that the stress-energy tensor is divergence-less due to the particles, fluids, fields ... equations of motion and in the last equality the killing equation and the symmetry of the stress-energy tensor. We may also define as many scalar quantities, for each α

$$Q(\alpha) = \int_{t=\text{constant}} J^\mu(\alpha) d^3\Sigma_\mu = \int J^0(\alpha) dx dy dz. \quad (5.13)$$

such that

$$\frac{dQ(\alpha)}{dt} = \int J^0_{,0} dx dy dz = - \int J^k_{,k} dx dy dz = - \int_{\text{closed surface}} J^k d^2S_k = 0, \quad (5.14)$$

where in the second equality we used Eq. (5.12), in the third equality we used Gauss theorem, and in the last equality we used the fact that there is no current source within the closed surface. The we see that the 10 scalars $Q(\alpha)$ are *conserved quantities*.

So we will have explicitly:

i. for $\vec{\xi} = \partial/\partial t$

$$\int J^0 d^3\mathbf{x} = \int T^{00} d^3\mathbf{x} = \text{constant}, \quad (5.15)$$

which is the conservation of total mass-energy.

ii. for the 3 $\vec{\xi} = \partial/\partial x^k$

$$\int J^0 d^3\mathbf{x} = - \int T^{0k} d^3\mathbf{x} = \text{constant}, \quad (5.16)$$

which is the conservation of the k -component of the momentum density.

iii. for $\vec{\xi} = x\partial/\partial y - y\partial/\partial x$

$$\int J^0 d^3\mathbf{x} = - \int (xT^{02} - yT^{01}) d^3\mathbf{x} = \text{constant}, \quad (5.17)$$

which is the conservation of the z component of the angular momentum density. The same holds for the other 2 components.

iv. for $\vec{\xi} = x\partial/\partial t + t\partial/\partial x$

$$\int J^0 d^3\mathbf{x} = \int (xT^{00} - tT^{0x}) d^3\mathbf{x} = \text{constant}. \quad (5.18)$$

The same holds for the other 2 boosts along y and z . If we define

$$x_{\text{c.m.}} = \frac{\int xT^{00} d^3\mathbf{x}}{\int T^{00} d^3\mathbf{x}}, \quad v_{\text{c.m.}}^x = \frac{\int T^{0x} d^3\mathbf{x}}{\int T^{00} d^3\mathbf{x}}, \quad (5.19)$$

then the conservation laws (5.18) tells that the center of mass has uniform motion along the x direction

$$x_{\text{c.m.}} = v_{\text{c.m.}}^x t + \text{constant}. \quad (5.20)$$

Globally conserved quantities

Imagine we found a killing vector $\vec{\xi}$ then the current $J^\mu = T^{\mu\nu}\xi_\nu$ is certainly covariantly constant $J^\mu{}_{;\mu} = 0$, since the stress-energy tensor is covariantly constant and symmetric and the killing equation 5.1 holds. Integrating then on a region Ω of spacetime

$$0 = \int_\Omega J^\mu{}_{;\mu} \sqrt{|g|} d^4\vec{x} = \int_\Omega (\sqrt{|g|}J^\mu)_{;\mu} d^4\vec{x} = \int_{\text{time } t_2} J^\mu d^3\Sigma_\mu - \int_{\text{time } t_1} J^\mu d^3\Sigma_\mu, \quad (5.21)$$

where in the third equality we used Gauss theorem. So the scalar quantity

$$Q = \int_{t=\text{constant}} J^\mu d^3\Sigma_\mu, \quad (5.22)$$

is conserved.

Internal symmetries

We saw in Eq. (5.18) that in a LLF

$$J^{\alpha\beta}(0) = \int_{t=\text{constant}} (x^\alpha T^{\beta\gamma} - x^\beta T^{\alpha\gamma}) d^3\Sigma_\gamma, \quad (5.23)$$

is the conserved total angular momentum density about the origin. So we may define a tensor

$$J^{\alpha\beta\gamma} = x^\alpha T^{\beta\gamma} - x^\beta T^{\alpha\gamma}, \quad (5.24)$$

and prove that $J^{\alpha\beta\gamma}{}_{;\gamma} = 0$ by going into an inertial LLF (so that $;\rightarrow ,$) and using the symmetry of the stress-energy tensor. Analogously we may define the conserved total angular momentum density about an event \vec{c} as

$$\begin{aligned} J^{\alpha\beta}(c) &= J^{\alpha\beta}(0) - c^\alpha \int_{t=\text{constant}} T^{\beta\gamma} d^3\Sigma_\gamma + c^\beta \int_{t=\text{constant}} T^{\alpha\gamma} d^3\Sigma_\gamma \\ &= J^{\alpha\beta}(0) - c^\alpha p^\beta + c^\beta p^\alpha, \end{aligned} \quad (5.25)$$

where p^μ is the conserved 4-momentum density defined in (5.15) and (5.16). But we note that $J^{\alpha\beta}$ is not invariant under this coordinate transformation.

In order to define “an angular momentum” that is invariant under the coordinate transformation, i.e. the *internal angular momentum* or *spin* we may define $S^{\alpha\beta}$ as $J^{\alpha\beta}$ about points on the center of mass worldline.

While this program can always be carried out in an inertial LLF, i.e. in special relativity, it is not globally on the whole spacetime manifold, i.e. in general relativity. In fact in general relativity there may exist no killing vector and one cannot in general define $J^{\alpha\beta}$. This can be done only for *isolated* gravitating systems or for *small* objects.

VI. IN QUANTUM FIELD THEORY [8]

Consider a *linear global symmetry* like the one considered in Noether theorem IV.2

$$\varphi'_i(x') = R_{ij}(\mathbf{g})\varphi_j(x) \quad (6.1)$$

where the group element \mathbf{g} does not depend on the spacetime variable x . As for Noether theorem we explore the consequences of invariance only under infinitesimal group transformations

$$\delta\varphi_i(x) = M_{ij}^a\varphi_j(x)\delta\omega^a, \quad (6.2)$$

in which $\delta\omega^a$ are infinitesimal parameters independent of x . From the discussion in Section VI we require that

$$\delta_a S = \delta\omega^a \int M_{ij}^a\varphi_j(x) \frac{\delta S}{\delta\varphi_i(x)} dx = 0, \quad (6.3)$$

where we denote with $\delta/\delta\varphi(x)$ a functional derivative.

A. Ward-Takahashi identities [9]

We now consider the generating functional of correlation functions $Z[J]$ corresponding to the symmetric action S

$$Z[J] = \int \exp \left[iS + \int J_i(x)\varphi_i(x) dx \right] \mathcal{D}\varphi(x). \quad (6.4)$$

We here want to discuss the consequences of Eq. (6.3). Since the action S is left invariant and the source term gives a contribution $\int J_i(x)M_{ij}^a\varphi'_j(x)\delta\omega^a$ we may write

$$0 = \delta_a Z[J] = \delta\omega^a \int \mathcal{D}\varphi(x) \int dx J_i(x)M_{ij}^a\varphi_j(x) \exp \left[iS + \int J_i(x)\varphi_i(x) dx \right], \quad (6.5)$$

where, since we want to neglect infinitesimal terms of order higher than the first, the Jacobian of the measure of integration has to be taken simply as 1, and we have renamed $\varphi'_i(x)$ as $\varphi_i(x)$ since the integration variable in the path integral is dummy.

Since Eq. (6.5) must hold for any $\delta\omega^a$, it can be rewritten for each component a . Finally the identity

$$\int \varphi_i(x) \exp \left[iS + \int J_k(x)\varphi_k(x) dx \right] \mathcal{D}\varphi(x) = \frac{\delta}{\delta J_i(x)} \int \exp \left[iS + \int J_k(x)\varphi_k(x) dx \right] \mathcal{D}\varphi(x) \quad (6.6)$$

allows to rewrite Eq. (6.5) as an equation for the functional $Z[J]$

$$\int M_{ij}^a J_i(x) \frac{\delta Z[J]}{\delta J_j(x)} dx = 0. \quad (6.7)$$

This equation immediately implies an identical equation for the generating functional $W[J] = \ln Z[J]$ of connected correlation functions

$$\int M_{ij}^a J_i(x) \frac{\delta W[J]}{\delta J_j(x)} dx = 0. \quad (6.8)$$

Expanding this equation in a power series of the source $J(x)$, we obtain identities between the connected correlation functions which describe the physical implications of the symmetry of the action.

VII. SUM RULES

A. Atom [10]

In considering the interaction of an electromagnetic field with an atom it is often necessary to evaluate matrix elements of tensor operators with respect to angular momentum eigenstates (see Appendix B). Examples are the Stark or the Zeeman effects. In general it is a formidable task to calculate such matrix elements. However, there are certain properties of these matrix elements that follow purely from geometric considerations.

Wigner-Eckart theorem

The Wigner-Eckart theorem is one of the most important theorems in Quantum Mechanics in this respect.

Theorem VII.1 (Wigner-Eckart). *Given a tensor operator $T^{(k)}$ and two states of angular momenta j and j' , there exists a constant $\langle j || T^{(k)} || j' \rangle$ such that for all m, m' , and q , the following equation is satisfied:*

$$\langle j m | T_q^{(k)} | j' m' \rangle = \langle j' m' k q | j m \rangle \langle j || T^{(k)} || j' \rangle, \quad (7.1)$$

where $T_q^{(k)}$ is the q -th component of the spherical tensor operator, $T^{(k)}$ of rank k , $|jm\rangle$ denotes an eigenstate of total angular momentum J^2 and its z component J_z , $\langle j' m' k q | j m \rangle$ is the Clebsch-Gordan coefficient for coupling j' with k to get j , $\langle j || T^{(k)} || j' \rangle$ denotes some value that does not depend on m, m' , nor q and is referred to as the reduced matrix element.

Selection rules

From the Wigner-Eckart theorem (7.1) follows that:

- i. A tensor operator of rank 0, i.e. a scalar $T_0^{(0)}$, cannot change j, m values;
- ii. A vector operator is a spherical tensor of rank 1 so that only $\Delta m = m - m' = \pm 1, 0$ and $\Delta j = j - j' = \pm 1, 0$ are possible. In addition the $j = 0 \rightarrow 0$ transition is forbidden. This selection rule is of fundamental importance in the theory of radiation. It is the dipole selection rule obtained in the long wavelength limit of emitted photons.
- iii. There is a very simple m -selection rule

$$\langle j m | T_q^{(k)} | j' m' \rangle = 0, \quad \text{unless} \quad m = q + m'. \quad (7.2)$$

B. Atomic [11] and Coulombic [12] Liquid

In the theory of a Coulomb [20] and an Atomic [21] liquid the normalization condition of certain static and dynamic n -body correlation functions or their properties stemming from the Born-(Bogoliubov)-Green-(Kirkwood)-Yvon (B(B)G(K)Y static and dynamic (.)) structure equations give rise to a series of sum rules that must be fulfilled exactly within certain weak hypotheses. In this section we will denote with \mathbf{r} a point in space. Moreover we work in imaginary time β which represents the inverse temperature at which the liquid is in thermal equilibrium.

Static structure

The (static) BGY structure equations hold in any statistical ensemble [11, 22, 23]: canonical, grand canonical,

Coulomb liquid

Consider a mixture of s species of positive and negative point ions with charges e_α , $\alpha = 1, 2, \dots, s$ in thermal equilibrium at an inverse temperature $\beta = 1/k_B T$ with k_B Boltzmann constant. They will interact pairwise through the Coulomb potential $\phi^c(\mathbf{r})$, the solution of the Poisson equation in dimension $d = 1, 2, 3$

$$\Delta \phi^C(\mathbf{r}) = -\varepsilon_d \delta^d(\mathbf{r}), \quad \varepsilon_d = \begin{cases} 4\pi & d = 3 \\ 2\pi & d = 2 \\ 2 & d = 1 \end{cases}, \quad (7.3)$$

where δ^d is a d -dimensional Dirac delta function. Namely

$$\phi^C(\mathbf{r}) = \begin{cases} 1/|\mathbf{r}| & d = 3 \\ -\ln(|\mathbf{r}|/\ell) & d = 2 \\ -|\mathbf{r}| & d = 1 \end{cases} \quad (7.4)$$

where ℓ is a parameter of the dimension of length. For the Coulomb potential on a Riemannian surface see Ref. [24–26].

Define the local density and charge of particles of species α

$$N(\alpha, \mathbf{r}) = \sum_j \delta_{\alpha, \alpha_j} \delta(\mathbf{r} - \mathbf{r}'_j), \quad (7.5)$$

$$C(\mathbf{r}) = \sum_\alpha e_\alpha N(\alpha, \mathbf{r}). \quad (7.6)$$

The multipolar sum rules

$$\int d\mathbf{r} \mathcal{Y}_l(\mathbf{r}) \langle C(\mathbf{r}) A(\mathbf{a}) \rangle_T = 0, \quad (7.7)$$

where A is a localized observable, $\langle C(\mathbf{r}) A \rangle_T = \langle C(\mathbf{r}) A \rangle - \langle C(\mathbf{r}) \rangle \langle A \rangle$ is the truncated thermal average defined for an infinitely extended system neglecting any finite-size effects, and $\mathcal{Y}_l(\mathbf{r}) = r^l P_l(\cos\theta)$ is the harmonic polynomial of order $l = 0, 1, 2, \dots$, with P_l the usual Legendre polynomials of order l and θ the polar angle for \mathbf{r} .

Choosing $A = N(\alpha_1, \mathbf{r}_1) \cdots N(\alpha_n, \mathbf{r}_n)$ in (7.7) gives the (l, n) multipolar sum rule that tells that the excess charge density,

$$c(\mathbf{r} | \alpha_1, \mathbf{r}_1, \dots, \alpha_n, \mathbf{r}_n) = \sum_\alpha e_\alpha \rho_T(\alpha, \mathbf{r} | \alpha_1, \mathbf{r}_1, \dots, \alpha_n, \mathbf{r}_n), \quad (7.8)$$

with

$$\rho_T(\alpha, \mathbf{r} | \alpha_1, \mathbf{r}_1, \dots, \alpha_n, \mathbf{r}_n) = \langle N(\alpha, \mathbf{r}) [N(\alpha_1, \mathbf{r}_1) \cdots N(\alpha_n, \mathbf{r}_n)]_{\text{DP}} \rangle - \langle N(\alpha, \mathbf{r}) \rangle \langle [N(\alpha_1, \mathbf{r}_1) \cdots N(\alpha_n, \mathbf{r}_n)]_{\text{DP}} \rangle, \quad (7.9)$$

where [DP] stands for different particles, i.e. $\mathbf{r}_1 \neq \mathbf{r}_2 \neq \dots \neq \mathbf{r}_n$, does not carry multipoles of any order.

We will also define the truncated (Ursell) correlation functions as

$$\rho_T(\alpha_1, \mathbf{r}_1, Q) = \rho(\alpha_1, \mathbf{r}_1, Q) - \rho(\alpha_1, \mathbf{r}_1) \rho(Q), \quad (7.10)$$

$$\rho_T(\alpha, \mathbf{r}, \alpha_1, \mathbf{r}_1, Q) = \rho(\alpha, \mathbf{r}, \alpha_1, \mathbf{r}_1, Q) - \rho(\alpha_1, \mathbf{r}_1) \rho_T(\alpha, \mathbf{r}, Q) - \rho(\alpha, \mathbf{r}) \rho_T(\alpha_1, \mathbf{r}_1, Q) - \rho(Q) \rho_T(\alpha, \mathbf{r}, \alpha_1, \mathbf{r}_1), \quad (7.11)$$

where $Q = (q_2, \dots, q_n)$ with $q = (\alpha, \mathbf{r})$ and

$$\rho(\alpha_1, \mathbf{r}_1, \dots, \alpha_n, \mathbf{r}_n) = \langle [N(\alpha_1, \mathbf{r}_1), \dots, N(\alpha_n, \mathbf{r}_n)]_{\text{DP}} \rangle. \quad (7.12)$$

A simple argument based on the harmonicity of the Coulomb potential shows that all types of asymptotic behavior are not possible in a homogeneous classical charged fluid: if the truncated correlations are integrable and monotonously decreasing at infinity, they have to decay faster than any inverse power.

Clustering

Theorem VII.2 (Coulomb clustering [12]). *If the correlations satisfy BGY equations. Assume $e_{\alpha_1}e_{\alpha_2}\rho_T(\alpha_1, \mathbf{r}, \alpha_2, \mathbf{0}) < 0$ at sufficiently large r and $\rho_T(\alpha_1, \mathbf{r}, \alpha_2, \mathbf{0})$ is integrable and tends monotonously to zero as $r \rightarrow \infty$. Moreover for r large enough, $|\rho_T(\alpha, \mathbf{r}, \alpha', \mathbf{r}', \mathbf{0})| \leq M(t)|\rho_T(\alpha, r)|$, $t = \min(|\mathbf{r} - \mathbf{r}'|, |\mathbf{r}'|)$, and $\lim_{t \rightarrow \infty} M(t) = 0$, then $\lim_{r \rightarrow \infty} r^p \rho_T(\alpha, r) = 0$ for all $p > 0$.*

This tells that among all pair potential between the particles of a liquid the Coulomb is the only one for which we must have clustering faster than any inverse power (see also section II.B.3 of Ref. [12]). if the structure function of the homogeneous plasma does not decay faster than any inverse power, it must either have oscillations, or be nonintegrable. We cannot exclude an oscillatory behavior as $\cos(\lambda r)/r^p$.

Multipolar sum rules

Theorem VII.3 (multipolar sum-rules [12]). *Let the space dimension d be two or three. If the correlations satisfy BGY equations and*

$$|d^n \rho_T(\alpha_1, \mathbf{r}_1, \dots, \alpha_n, \mathbf{r}_n)| \leq M, \quad d = \sup_{i,j} |\mathbf{r}_i - \mathbf{r}_j|, \quad (7.13)$$

for $\eta > d + l_0$ and $n = 2, \dots, n_0 + 2$ then the (l, n) multipolar sum rules (7.7) hold for $l \leq l_0, n \leq n_0$.

Stillinger-Lovett second moment sum rule

Theorem VII.4 (Stillinger-Lovett sum rule [12]). *If the charge ($l = 0$) and dipole ($l = 1$) sum rules (7.7) are verified for $n = 1, 2$ and if*

$$\int dq_1 \int dq_2 |\mathbf{r}_2| |\rho_T(q_1, q_2, q)| < \infty, \quad (7.14)$$

then the following second moment condition holds

$$\beta \int d\mathbf{r}' \int d\mathbf{r} \frac{S(\mathbf{r})}{|\mathbf{r} - \mathbf{r}'|} = 1, \quad (7.15)$$

$$S(\mathbf{r} - \mathbf{r}') = S(\mathbf{r}|\mathbf{r}') = \langle C(\mathbf{r})C(\mathbf{r}') \rangle - \langle C(\mathbf{r}) \rangle \langle C(\mathbf{r}') \rangle, \quad (7.16)$$

where $S(\mathbf{r})$ is known as the static structure factor. Applying the convolution theorem of Fourier transforms, this is equivalent to

$$2\pi(d-1)\beta \lim_{|\mathbf{k}| \rightarrow 0} \frac{\tilde{S}(\mathbf{k})}{|\mathbf{k}|^2} = 1, \quad (7.17)$$

where $\tilde{S}(\mathbf{k}) = \int d\mathbf{r} e^{i\mathbf{k} \cdot \mathbf{r}} S(\mathbf{r})$ and $2\pi(d-1)|\mathbf{k}|^{-2}$ is the Fourier transform of the Coulomb potential (7.4) in dimension $d = 2, 3$. Alternatively, expanding $S(\mathbf{k})$ to second order in \mathbf{k} around $\mathbf{k} = \mathbf{0}$ and using spherical symmetry

$$\beta \int d\mathbf{r} |\mathbf{r}_j|^2 S(\mathbf{r}) = \frac{\beta}{d} \int d\mathbf{r} |\mathbf{r}|^2 S(\mathbf{r}) = -\frac{1}{\pi(d-1)}, \quad j = 1, 2, \dots, d. \quad (7.18)$$

$$(7.19)$$

Note that in a homogeneous and isotropic fluid $S(\mathbf{r}) = S(|\mathbf{r}|)$ and the only non-zero moments are the even ones. The zero moment being the charge sum rule $\tilde{S}(\mathbf{0}) = 0$ which corresponds to the screening of an *internal* charge [22]¹⁰ whereas the second moment sum rule above corresponds to the screening of an *external* charge. For the fourth moment sum rule see Refs. [23, 27].

¹⁰ In Ref. [22] is also shown the relation between the static structure factor \tilde{S} and the internal dipole sum rule.

The Stillinger-Lovett sum rule above is equivalent to the property of the vanishing in the limit of small wave numbers of the inverse dielectric function

$$\epsilon^{-1}(\mathbf{k}) = 1 - 2\pi(d-1)\beta \frac{\tilde{S}(\mathbf{k})}{|\mathbf{k}|^2}, \quad (7.20)$$

obtained from the response of the liquid to an external spatially modulated charge density. When the conditions (7.18), (7.17), or (7.15) hold, the liquid completely shields any external charge inhomogeneity and behaves as a conducting medium.

Atomic liquid

In this case we may choose all $e_\alpha = 1$ for any one of the s species of the liquid mixture. Moreover the interaction potential is non Coulombic but the one of Lennard-Jones [11] which combines a repulsive potential, $1/r^n$, with an attractive potential, $-1/r^m$, using empirically determined coefficients A_n and B_m [28, 29]

$$\phi^{\text{LJ}}(\mathbf{r}) = \frac{A_n}{r^n} - \frac{B_m}{r^m}. \quad (7.21)$$

In his 1931 review [29] Lennard-Jones suggested using $m = 6$ to match the London dispersion force and $n = 12$ based matching experimental data. Setting $A_n = 4\epsilon\sigma^{12}$ and $B_m = 4\epsilon\sigma^6$ gives the widely used Lennard-Jones 12-6 potential.

Now the clustering will follow an inverse power law (see also section II.B.3 of Ref. [12]) and the multipolar sum rules will not be valid anymore. Except for the charge sum rule that will continue to hold since it is just a normalization condition of the correlation functions according to

$$\int d\mathbf{r}_1 d\mathbf{r}_2 \cdots d\mathbf{r}_n \rho(\mathbf{r}_1, \dots, \mathbf{r}_n) = \frac{N!}{(N-n)!}, \quad (7.22)$$

that follows directly from the definition (7.12) in the canonical ensemble. In particular this also implies that

$$\tilde{S}(\mathbf{0}) = 0. \quad (7.23)$$

Note that in this case [30]

$$\lim_{|\mathbf{r}| \rightarrow \infty} \frac{\rho(\mathbf{r}, \mathbf{r}')}{\rho(\mathbf{r})\rho(\mathbf{r}')} = 1 - \frac{\chi_T}{\chi_T^0} \frac{1}{N} + o(1/N), \quad (7.24)$$

where $\chi_T = [\rho(\partial P / \partial \rho)_{N,T}]^{-1}$ is the isothermal compressibility of the fluid, and $\chi_T^0 = \beta / \rho$ is the isothermal compressibility of the ideal gas. Moreover one should keep in mind that in the canonical ensemble the isothermal compressibility must vanish since N, V, T are kept constant. So one really finds $\lim_{r \rightarrow \infty} g(r) = 1 - 1/N$ which is the ideal gas result for the asymptotic behavior of the radial distribution function $g(|\mathbf{r} - \mathbf{r}'|) = \rho(\mathbf{r}, \mathbf{r}') / \rho(\mathbf{r})\rho(\mathbf{r}')$.

On the other hand, in the grand canonical ensemble, where $P(N)$ is the probability that the fluid contains N particles irrespective of their coordinates and momenta, we define instead

$$\rho_{\text{gc}}(\mathbf{r}_1, \dots, \mathbf{r}_n) = \sum_{N \geq n} P(N) \rho(\mathbf{r}_1, \dots, \mathbf{r}_n), \quad (7.25)$$

where $P(N) = \exp(N\beta\mu)Q_N / \Theta$ with $\Theta = \exp(\beta PV) = \sum_{N=0}^{\infty} \exp(N\beta\mu)Q_N$, with P the pressure, V the volume of the liquid, μ is the chemical potential, and Q_N is the canonical partition function of the fluid of $N = \rho V$ particles. Then the ρ_{gc} are normalized as $\int \rho_{\text{gc}}(\mathbf{r}_1, \dots, \mathbf{r}_n) d\mathbf{r}_1 \cdots d\mathbf{r}_n = \langle N! / (N-n)! \rangle_\mu$, where $\langle \dots \rangle_\mu$ denotes an average with respect to $P(N)$.

The average number of particles in the system is

$$\langle N \rangle_\mu = \sum_{N=0}^{\infty} N P(N) = \frac{\partial \ln \Theta}{\partial \beta \mu}, \quad (7.26)$$

so that

$$\frac{\partial \langle N \rangle_\mu}{\partial \beta \mu} = \langle N^2 \rangle_\mu - \langle N \rangle_\mu^2. \quad (7.27)$$

It follows then

$$0 \leq \frac{\langle N^2 \rangle_\mu - \langle N \rangle_\mu^2}{\langle N \rangle_\mu} = \frac{1}{\langle N \rangle_\mu} \frac{\partial \langle N \rangle_\mu}{\partial \beta \mu}, \quad (7.28)$$

where this intensive ratio is related to the isothermal compressibility. In fact, for an infinitesimal isothermal change it follows that $VdP = Nd\mu$, where P is the pressure. If the change also takes place at constant volume, both dP and $d\mu$ are proportional to dN : $dP = (\partial P/\partial N)_{V,T}dN$ and $d\mu = (\partial \mu/\partial N)_{V,T}dN$. So that $N(\partial \mu/\partial N)_{V,T} = V(\partial P/\partial N)_{V,T} = (\partial P/\partial \rho)_{N,T} = 1/\rho\chi_T$, with χ_T the isothermal compressibility. In the thermodynamic limit N may be replaced by $\langle N \rangle_\mu$ so that [11]

$$\frac{\langle N^2 \rangle_\mu - \langle N \rangle_\mu^2}{\langle N \rangle_\mu} = \frac{\rho\chi_T}{\beta} = \frac{\chi_T}{\chi_T^0}, \quad (7.29)$$

with χ_T^0 the isothermal compressibility of the ideal gas.

From the normalization condition for ρ_{gc} and the thermodynamic condition of Eq. (7.28), it follows immediately that, if the system is homogeneous, i.e. ρ_{gc} is constant and equal to $\rho = \langle N \rangle/V$,

$$\begin{aligned} \tilde{S}_{gc}(\mathbf{0}) &= 1 + \rho \int [g_{gc}(r) - 1] d\mathbf{r} \\ &= 1 + \frac{\langle N(N-1) \rangle_\mu}{V\rho} - \langle N \rangle_\mu \\ &= \frac{\langle N^2 \rangle_\mu}{\langle N \rangle_\mu} - \langle N \rangle_\mu = \frac{\chi_T}{\chi_T^0}. \end{aligned} \quad (7.30)$$

Comparing Eq. (7.30) with Eq. (7.23) we then see that the structure predicted by the canonical ensemble does not agree with the one predicted by the grand canonical ensemble for long range (unscreened) Coulomb fluids. They do give rise to ensemble inequivalence¹¹. For short range or long range non Coulombic systems one should study case by case.

At criticality

On approaching a phase transition [33–36] some sum rules will merge and some will cease to hold. In particular, once a description in terms of an order parameter is found, we may end up with a unified treatment of sum rules and upon the divergence of certain correlation lengths some other may fail. We will call this process the “melting or evaporation of the sum rules”. An example of failure is given by the second and fourth moment sum rules for ionic liquids at their vapor-liquid phase transition [36]. The universality property of the renormalization group is an indication of the mathematical unification of similar sum rules but holding in different physical systems.

Dynamic structure

Linear response theory [11, 20, 21] is a well known framework to describe the approach to thermal equilibrium in response to an external perturbation acting on a many-body quantum fluid. Our discussion is rather general and valid for a quantum fluid¹².

Let us introduce the density linear response function $K(\mathbf{r} - \mathbf{r}', t - t')$ for a homogeneous fluid. Let us indicate with V_b the “bare” potential in vacuum.

The coupling of the fluid to the perturbing potential is described by the Hamiltonian

$$H'(t) = \int d\mathbf{r} \rho(\mathbf{r}) V_b(\mathbf{r}, t), \quad (7.31)$$

¹¹ Here we are thinking of unscreened charged liquids, i.e. liquids whose constituents particles are (not completely screened) charges. Not liquids like water or even like ionic screened two component liquids where one should rather look at the Bhatia-Thornton structure factors as done in Refs. [31–33]. In particular the work of Aqua and Fisher [33] suggests to look for ensemble inequivalence in ionic liquids near the critical point when there is a *ionic asymmetry* which couples charge and density fluctuations in a direct manner: The charge correlation length then diverges precisely as the density correlation length.

¹² The same arguments can be translated in terms of a classical fluid upon substituting the commutator $[\cdot, \cdot]$ with a Poisson bracket $\{\cdot, \cdot\}$ [11].

where $\rho(\mathbf{r})$ is the density operator (here we implicitly assume that the mean value of the density has been subtracted from $\rho(\mathbf{r})$). We will just consider the linear effect of this perturbation. The change in density is given by

$$\delta n(\mathbf{r}, t) = \langle \rho(\mathbf{r}) \rangle - \langle \rho(\mathbf{r}) \rangle_0 = \text{tr}\{[w(t) - w_0]\rho(\mathbf{r})\}, \quad (7.32)$$

where tr denotes the trace, $w(t) = \int \psi^*(R, t)\psi(R, t) d^{3N}R$ is the perturbed density matrix whose unperturbed counterpart is $w_0 = \exp(-\beta H_0)/\text{tr}\{\exp(-\beta H_0)\}$, and $\beta = 1/k_B T$ with k_B the Boltzmann constant and T the absolute temperature. We are indicating with $\psi(R, t)$ the many-body wave function of the fluid with particles at positions $R = (\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_N)$ at time t . This satisfies to the Schrödinger equation

$$i\hbar \frac{\partial \psi(R, t)}{\partial t} = [H_0 + H'(t)]\psi(R, t), \quad (7.33)$$

where H is the Hamiltonian of the unperturbed fluid. Then the perturbed density matrix satisfies to

$$\begin{aligned} i\hbar \frac{\partial w(t)}{\partial t} &= [H_0 + H'(t), w(t)] \\ &\approx [H_0, w(t) - w_0] + [H'(t), w_0], \end{aligned} \quad (7.34)$$

where $[A, B]$ denotes the commutator $AB - BA$ and in the last step we have linearized the effect of the perturbation and used $[H_0, w_0] = 0$. This equation is subject to the initial condition

$$\lim_{t \rightarrow -\infty} w(t) = w_0, \quad (7.35)$$

representing a state of thermal equilibrium.

The linearized equation (7.34) has the following solution

$$w(t) - w_0 = (i\hbar)^{-1} \int_{-\infty}^t dt' \exp\{-iH_0(t-t')/\hbar\} [H'(t'), w_0] \exp\{iH_0(t-t')/\hbar\}. \quad (7.36)$$

Inserting this result into Eq. (7.32) and using the cyclic invariance of the trace, $\text{tr}\{AB\} = \text{tr}\{BA\}$, we can write the desired result as follows

$$\delta n(\mathbf{r}, t) = (-i/\hbar) \int d\mathbf{r}' \int_{-\infty}^t dt' \langle [\rho(\mathbf{r}, t), \rho(\mathbf{r}', t')] \rangle_0 V_b(\mathbf{r}', t). \quad (7.37)$$

Again the angle parenthesis $\langle A \rangle_0 = \text{tr}\{w_0 A\}$ denotes the mean value on the equilibrium state and $\rho(\mathbf{r}, t)$ is the Heisenberg operator

$$\rho(\mathbf{r}, t) = \exp(iH_0 t/\hbar) \rho(\mathbf{r}) \exp(-iH_0 t/\hbar). \quad (7.38)$$

So

$$K(\mathbf{r} - \mathbf{r}', t - t') = (-i/\hbar) \theta(t - t') \langle [\rho(\mathbf{r}, t), \rho(\mathbf{r}', t')] \rangle_0. \quad (7.39)$$

This result clearly embodies the causality property through the Heaviside step function θ .

Introducing the notation

$$\chi''(k, t - t') = (1/2\hbar) \int d(\mathbf{r} - \mathbf{r}') \exp[-i\mathbf{k} \cdot (\mathbf{r} - \mathbf{r}')] \langle [\rho(\mathbf{r}, t), \rho(\mathbf{r}', t')] \rangle_0, \quad (7.40)$$

we see, from Eq. (7.39) that the Fourier transform of K is the convolution integral of the Fourier transform of $\chi''(k, t)$, that we will indicate with $\chi''(k, \omega)$, and of the Heaviside step function, that is equal to $i/(\omega + i\eta)$ with η a small positive quantity. We can then write the space-time Fourier transform of K like so

$$\chi(k, \omega) = - \int_{-\infty}^{\infty} \frac{d\omega'}{\pi} \chi''(k, \omega') / (\omega - \omega' + i\eta). \quad (7.41)$$

Using the rule $(\omega + i\eta)^{-1} = P(1/\omega) - i\pi\delta(\omega)$, where P denotes the Cauchy principal part, this can be written like so

$$\chi(k, \omega) = -P \int_{-\infty}^{\infty} \frac{d\omega'}{\pi} \chi''(k, \omega') / (\omega - \omega') + i\chi''(k, \omega). \quad (7.42)$$

Since $\chi''(k, t)$ is written in terms of the commutator of Hermitian operators it can be readily shown that $\chi''(k, \omega)$ must be real. So we can write

$$\text{Im}\chi(k, \omega) = \chi''(k, \omega). \quad (7.43)$$

Fluctuation-dissipation theorem

We now worry about the relationship between the density response function and the van Hove dynamic response $S(\mathbf{k}, \omega)$. Let us define the autocorrelation density function as

$$G(\mathbf{r} - \mathbf{r}', t - t') = \frac{1}{n} \langle \rho(\mathbf{r}, t) \rho(\mathbf{r}', t') \rangle_0, \quad (7.44)$$

whose space-time Fourier transform is $S(\mathbf{k}, \omega)$. The connection between G e K that gush from Eq. (7.39) can be rewritten in Fourier transform like so

$$\chi(\mathbf{k}, \omega) = (n/\hbar) \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} [S(\mathbf{k}, \omega) - S(-\mathbf{k}, -\omega)] / (\omega - \omega' + i\eta). \quad (7.45)$$

This has the same form of Eq. (7.41) so that

$$\text{Im}\chi(\mathbf{k}, \omega) = (-n/2\hbar)[S(\mathbf{k}, \omega) - S(-\mathbf{k}, -\omega)]. \quad (7.46)$$

For a fluid in thermodynamic equilibrium we must have

$$S(-\mathbf{k}, -\omega) = \exp(-\hbar\beta\omega)S(\mathbf{k}, \omega). \quad (7.47)$$

In order to prove this property we observe that its inverse space-time Fourier transform reads

$$G(-\mathbf{r}, -t) = \exp\left(-i\hbar\beta\frac{\partial}{\partial t}\right) G(\mathbf{r}, t), \quad (7.48)$$

since under time Fourier transform $\partial/\partial t \rightarrow -i\omega$. But Eq. (7.48) can readily be proven through the following steps (where, once again we use the cyclic invariance of the trace and the definition of the Heisenberg operator, Eq. (7.38))

$$\begin{aligned} \text{tr}\{\exp(-\beta H_0)\rho(\mathbf{0}, 0)\rho(\mathbf{r}, t)\} &= \text{tr}\{\rho(\mathbf{r}, t)\exp(-\beta H_0)\rho(\mathbf{0}, 0)\} \\ &= \text{tr}\{\exp(-\beta H_0)\rho(\mathbf{r}, t - i\hbar\beta)\rho(\mathbf{0}, 0)\} \\ &= \exp(-i\hbar\beta\partial/\partial t)\text{tr}\{\exp(-\beta H_0)\rho(\mathbf{r}, t)\rho(\mathbf{0}, 0)\}. \end{aligned} \quad (7.49)$$

In the classical limit, for β small, Eq. (7.46) becomes

$$\text{Im}\chi(\mathbf{k}, \omega) = (-n\beta\omega/2)S(\mathbf{k}, \omega). \quad (7.50)$$

Kramers-Kronig relations

Causality imposes that the response function $K(\mathbf{r}, t)$ vanish for $t < 0$. In other words the fluid is influenced only by the action of the external perturbation in the past. Introducing the “intermediate” response function $\chi(\mathbf{k}, t)$ as the space Fourier transform of $K(\mathbf{r}, t)$, we have

$$\chi(\mathbf{k}, t) = 0 \quad \text{for } t < 0. \quad (7.51)$$

On the other hand

$$\chi(\mathbf{k}, t) = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \exp(-i\omega t)\chi(\mathbf{k}, \omega). \quad (7.52)$$

Extending the definition of $\chi(\mathbf{k}, \omega)$ from real to complex frequencies, we can calculate this integral through contour methods and for $t < 0$ we can close the contour with the semicircle at infinity above the real axis. The contribution from the integration on the semicircle vanishes since $\chi(\mathbf{k}, \omega) \propto \omega^{-2}$ at high frequency. So the causality property (7.51) is guaranteed if $\chi(\mathbf{k}, \omega)$ is analytic in the upper part of the complex frequency plane.

Let us now consider the integral

$$\oint \frac{\chi(\mathbf{k}, \omega')}{\omega - \omega'} d\omega' = 0, \quad (7.53)$$

on the contour Γ shown in Fig. 5. This contour integral vanishes due to the analiticity of $\chi(\mathbf{k}, \omega)$. The contribution from the semicircle at infinity is again zero, so that

$$P \int_{-\infty}^{\infty} d\omega' \frac{\chi(\mathbf{k}, \omega')}{\omega' - \omega} - i\pi\chi(\mathbf{k}, \omega) = 0, \quad (7.54)$$

where again P denotes the Cauchy principal part of the integral on the real frequency axis and the second term comes from the integration over the small semicircle around the point ω . If we now separate $\chi(\mathbf{k}, \omega)$ into its real and imaginary parts we find

$$P \int_{-\infty}^{\infty} d\omega' \frac{\text{Re}\chi(\mathbf{k}, \omega')}{\omega' - \omega} + \pi \text{Im}\chi(\mathbf{k}, \omega) = 0, \quad (7.55)$$

and

$$P \int_{-\infty}^{\infty} d\omega' \frac{\text{Im}\chi(\mathbf{k}, \omega')}{\omega' - \omega} - \pi \text{Re}\chi(\mathbf{k}, \omega) = 0. \quad (7.56)$$

These are the Kramers-Kronig relations.

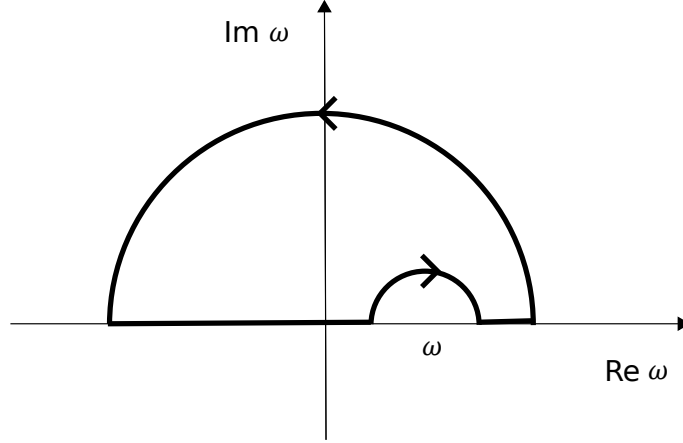


FIG. 5. Integration contour on the complex ω plane.

The dielectric function

In a Coulomb liquid, the connection with the longitudinal dielectric function $\epsilon(k, \omega)$, becomes apparent from the Poisson equations

$$\nabla \cdot \mathbf{D}(\mathbf{r}, t) = -4\pi e n_e(\mathbf{r}, t), \quad (7.57)$$

$$\nabla \cdot \mathbf{E}(\mathbf{r}, t) = -4\pi e [n_e(\mathbf{r}, t) + \delta n(\mathbf{r}, t)], \quad (7.58)$$

which yield

$$\frac{1}{\epsilon(k, \omega)} = \frac{\mathbf{k} \cdot \mathbf{E}(\mathbf{k}, \omega)}{\mathbf{k} \cdot \mathbf{D}(\mathbf{k}, \omega)} = 1 + \frac{\delta n(\mathbf{k}, \omega)}{n_e(\mathbf{k}, \omega)} = 1 + \frac{4\pi e^2}{k^2} \chi(k, \omega), \quad (7.59)$$

since from Eqs. (7.37) and (7.39) follows $\delta n(\mathbf{k}, \omega) = \chi(k, \omega) V_b(\mathbf{k}, \omega)$ where $\chi(k, \omega)$ is the Fourier transform of $K(|\mathbf{r} - \mathbf{r}'|, t - t')$ and

$$V_b(\mathbf{k}, \omega) = \frac{4\pi e^2}{k^2} n_e(\mathbf{k}, \omega). \quad (7.60)$$

Of course the field \mathbf{E} and the associated screened or “Hartree” potential $V_H(\mathbf{k}, \omega) = V_b(\mathbf{k}, \omega)/\epsilon(k, \omega)$ would be experienced by a second test charge introduced into the plasma, rather than by the particles of the plasma. The latter also experience effects which involve the precise “hole” a particle of the plasma digs around itself. This latter effect brings about the so called local field corrections.

In addition to $\chi(\mathbf{k}, \omega)$ which relates the displaced charge density to the potential *in vacuo*, it is useful to introduce yet another longitudinal response function, $\tilde{\chi}(k, \omega)$ say, by exploiting further the analogy with elementary electrostatics. This relates $n(\mathbf{k}, \omega)$ directly to the Hartree potential through

$$n(\mathbf{k}, \omega) = \tilde{\chi}(k, \omega) V_H(\mathbf{k}, \omega). \quad (7.61)$$

We then have

$$\epsilon(k, \omega) = 1 - \frac{4\pi e^2}{k^2} \tilde{\chi}(k, \omega). \quad (7.62)$$

The expression $\chi(k, \omega) = \tilde{\chi}(k, \omega)/\epsilon(k, \omega)$ accounts at one stroke for the *long range* effects of the Coulomb interactions (the resonance at the plasma frequency, determined by $\epsilon(k, \omega) = 0$, is brought about explicitly in the denominator).

The simplest useful approximation to the dielectric function of the plasma is obtained by approximating $\tilde{\chi}$ by the density response function of an ideal gas. This corresponds to the Vlasov theory for the classical plasma and to the Lindhard theory for the degenerate electron fluid. Refinements of these theories aims at incorporating the effects of “exchange and correlation” in $\tilde{\chi}$. This expression being an abbreviation for the short range effects arising from the statistics (“exchange”) and long range effect arising from the Coulomb interaction (“correlation”). Of course the exchange effects are absent in the classical limit.

Moments Sum Rules

Imagine we apply to the system H_0 a perturbation

$$H'(t) = \sum_{\alpha} \int d^2\mathbf{r} A_{\alpha}(\mathbf{r}) \lambda_{\alpha}(\mathbf{r}, t), \quad (7.63)$$

where $\lambda_{\alpha}(\mathbf{r}, t)$ are external fields and $A_{\alpha}(\mathbf{r})$ are observables of the system coupled to the fields. Our system now is $H = H_0 + H'$. We can then apply the formalism developed above in subsection “Dynamic structure” for the linear response theory.

Let us consider the moments of the dissipation spectrum, defined as

$$M_{\alpha\beta}^n(k) = - \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \omega^n \text{Im} \chi_{\alpha\beta}(k, \omega). \quad (7.64)$$

Since $\text{Im} \chi_{\alpha\beta}(k, \omega)$ is an odd function of ω due to Eq. (7.46), the even moments vanish. We will just be interested in the first two non-zero moments $n = 1, 3$. The moments are related to the fluctuations of the observables $A_{\alpha}(\mathbf{r})$ by the fluctuation-dissipation theorem in the following way

$$M_{\alpha\beta}^n(k) = - \frac{2}{(-i)^n} \left. \frac{\partial^n \chi_{\alpha\beta}''(k, t)}{\partial t^n} \right|_{t=0}, \quad (7.65)$$

$$\chi_{\alpha\beta}''(k, t) = - \frac{1}{2\hbar} \langle [A_{\alpha}(\mathbf{k}, t), A_{\beta}(-\mathbf{k}, 0)] \rangle_0, \quad (7.66)$$

where we used Eq. (7.43), $\langle \dots \rangle_0$ denotes the expectation value over the ground state of the unperturbed system H_0 , $[\cdot, \cdot]$ is the commutator, $A_{\alpha}(\mathbf{k}, t)$ is the Heisenberg representation of the spatial Fourier transform of $A_{\alpha}(\mathbf{r})$ such that

$$\frac{\partial A(t)}{\partial t} = [A(t), H_0]/i\hbar. \quad (7.67)$$

Let us write down the first two non-zero ones

$$M_{\alpha\beta}^1(k) = \frac{1}{\hbar^2} \langle [[A_{\alpha}, H_0], A_{\beta}] \rangle_0, \quad (7.68)$$

$$M_{\alpha\beta}^3(k) = \frac{1}{\hbar^4} \langle [[[[A_{\alpha}, H_0], H_0], H_0], A_{\beta}] \rangle_0, \quad (7.69)$$

where all the A observables are taken at $(k, 0)$.

Appendix A: Commutators

The commutator of two operators A and B is defined as

$$[A, B] = AB - BA. \quad (A1)$$

The commutator satisfies to the following Lie algebra relations

$$[A, A] = 0, \quad (\text{A2})$$

$$[A, B] = -[B, A], \quad (\text{A3})$$

$$[A, [B, C]] + [B, [C, A]] + [C, [A, B]] = 0, \quad (\text{A4})$$

where the third one is known as the Jacobi identity.

For three operators A, B , and C we also have

$$[A, B + C] = [A, B] + [A, C], \quad (\text{A5})$$

$$[A, BC] = B[A, C] + [A, B]C. \quad (\text{A6})$$

If $[A, B] = \alpha \in \mathbb{C}$ then

$$[A, B^2] = B[A, B] + [A, B]B = 2\alpha B, \quad (\text{A7})$$

$$[A, B^3] = B[A, B^2] + [A, B]B^2 = 3\alpha B^2, \quad (\text{A8})$$

$$\begin{aligned} & \dots \\ [A, B^n] &= n\alpha B^{n-1}. \end{aligned} \quad (\text{A9})$$

Then, given a smooth function f , using its Taylor series expansion, we readily obtain

$$[A, f(B)] = \alpha \frac{df(B)}{dB}. \quad (\text{A10})$$

In general we can prove the following lemma:

Theorem A.1 (Hadamard lemma). *Given any two operators A and B we have*

$$e^A B e^{-A} = B + [A, B] + \frac{1}{2!}[A, [A, B]] + \frac{1}{3!}[A, [A, [A, B]]] + \dots \quad (\text{A11})$$

Proof. Consider the function $f(s) = e^{sA} B e^{-sA}$. We want $f(1)$. Taylor expand $f(s)$ around $s = 0$

$$f(s) = f(0) + s f'(0) + \frac{1}{2!} s^2 f''(0) + \frac{1}{3!} s^3 f'''(0) + \dots, \quad (\text{A12})$$

but it is easy to see that

$$f'(s) = e^{sA} A B e^{-sA} - e^{sA} B A e^{-sA} = e^{sA} [A, B] e^{-sA}, \quad (\text{A13})$$

$$f''(s) = e^{sA} [A, [A, B]] e^{-sA}, \quad (\text{A14})$$

$$f'''(s) = e^{sA} [A, [A, [A, B]]] e^{-sA}, \quad (\text{A15})$$

and so on. \square

Another important result is the Baker–Campbell–Hausdorff formula:

Theorem A.2 (Baker–Campbell–Hausdorff formula). *Given any two operators A and B we have*

$$\ln(e^A e^B) = A + B + \frac{1}{2}[A, B] + \frac{1}{12}([A, [A, B]] + [B, [B, A]]) - \frac{1}{24}[B, [A, [A, B]]] + \dots \quad (\text{A16})$$

Proof. Consider

$$\frac{1}{1-x} = 1 + x + x^2 + x^3 + \dots \quad (\text{A17})$$

or

$$\frac{1}{1+x} = 1 - x + x^2 - x^3 + \dots \quad (\text{A18})$$

integrate respect to x

$$\ln(1+x) = x - \frac{1}{2}x^2 + \frac{1}{3}x^3 - \frac{1}{4}x^4 + \dots \quad (\text{A19})$$

or

$$\ln(x) = (x-1) - \frac{1}{2}(x-1)^2 + \frac{1}{3}(x-1)^3 - \frac{1}{4}(x-1)^4 + \dots \quad (\text{A20})$$

Now

$$\begin{aligned} \ln(e^A e^B) &= \sum_{k=1} \frac{(-1)^{k-1}}{k} \left(\sum_{m,n=0} \frac{A^m B^n}{m!n!} - 1 \right)^k \\ &= \left(A + B + AB + \frac{A^2 + B^2}{2} \dots \right) - \frac{1}{2} (A^2 + B^2 + AB + BA \dots) + \dots \\ &= A + B + \frac{1}{2}[A, B] + \dots \end{aligned} \quad (\text{A21})$$

□

Commutators are of fundamental importance in a *Lie algebra*: a vector space \mathfrak{g} together with an operation called the Lie bracket, an alternating bilinear map $\mathfrak{g} \times \mathfrak{g} \rightarrow \mathfrak{g}$, that satisfies the Jacobi identity. In other words, a Lie algebra is an algebra over a field for which the multiplication operation (called the Lie bracket) is alternating and satisfies the Jacobi identity. The Lie bracket of two vectors x and y is denoted $[x, y]$. A Lie algebra is typically a non-associative algebra. However, every associative algebra gives rise to a Lie algebra, consisting of the same vector space with the commutator Lie bracket, $[x, y] = xy - yx$.

Lie groups are smooth differentiable manifolds and as such can be studied using differential calculus, in contrast with the case of more general topological groups. One of the key ideas in the theory of Lie groups is to replace the global object, the group, with its local or linearized version, which Lie himself called its “infinitesimal group” and which has since become known as its Lie algebra or the tangent space to the manifold at the identity.

The following theorem is also of great importance:

Theorem A.3. *Given two hermitian operators A and B which commutes, $[A, B] = 0$, they can be diagonalized simultaneously on the same orthonormal basis of vectors of the Hilbert space.*

Proof. Thanks to the *spectral theorem* one can always find an orthonormal basis $\{e_i\}$ where A is diagonal. Then $Ae_i = \lambda_i e_i$ for each e_i . But from the hypothesis we also have $ABe_i = BAe_i = \lambda_i Be_i$ so Be_i is an eigenstate of A relative to the same eigenvalue λ_i . Then if the eigenvalue is non degenerate Be_i must be proportional to e_i . If the eigenvalue is degenerate one can always choose a linear combination of the basis of the subspace relative to it, \bar{e}_i such that it is a common eigenvector of A and B . □

Appendix B: Angular momentum

Consider the angular momentum hermitian operator $\hat{\mathbf{L}}$, where the hat denotes the operator. Then the following commutation relations hold

$$[\hat{L}_i, \hat{L}_j] = i\epsilon_{ijk} \hat{L}_k. \quad (\text{B1})$$

Then define

$$\hat{L}^2 = \sum_{i=1}^3 \hat{L}_i^2, \quad (\text{B2})$$

$$\hat{L}_{\pm} = \hat{L}_1 \pm i\hat{L}_2. \quad (\text{B3})$$

We can then prove the following relations

$$[\hat{L}^2, \hat{L}_i] = 0, \quad (\text{B4})$$

$$[\hat{L}_+, \hat{L}_-] = 2\hat{L}_3, \quad (\text{B5})$$

$$[\hat{L}_3, \hat{L}_{\pm}] = \pm \hat{L}_{\pm}, \quad (\text{B6})$$

and

$$\hat{L}^2 = \hat{L}_+ \hat{L}_- + \hat{L}_3^2 - \hat{L}_3 = \hat{L}_- \hat{L}_+ + \hat{L}_3^2 + \hat{L}_3 \quad (\text{B7})$$

Since \widehat{L}^2 commutes with \widehat{L}_3 we can diagonalize them simultaneously so that

$$\widehat{L}^2|\psi_{L,M}\rangle = \mathcal{L}^2|\psi_{L,M}\rangle, \quad (\text{B8})$$

$$\widehat{L}_3|\psi_{L,M}\rangle = M|\psi_{L,M}\rangle, \quad (\text{B9})$$

where, since $\widehat{L}^2 - \widehat{L}_3^2 = \widehat{L}_1^2 + \widehat{L}_2^2$, we called L the maximum value of $|M|$ for a given value \mathcal{L} . Then

$$\widehat{L}_3\widehat{L}_\pm|\psi_{L,M}\rangle = (M \pm 1)\widehat{L}_\pm|\psi_{L,M}\rangle, \quad (\text{B10})$$

$$\widehat{L}_+|\psi_{L,L}\rangle = 0. \quad (\text{B11})$$

From Eq. (B7) follows

$$0 = \widehat{L}_-\widehat{L}_+|\psi_{L,L}\rangle = (\widehat{L}^2 - \widehat{L}_3^2 - \widehat{L}_3)|\psi_{L,L}\rangle, \quad (\text{B12})$$

or $\mathcal{L}^2 = L(L+1)$. Also M can assume $2L+1$ values, namely $M = L, L-1, \dots, -L$. And $2L = 0, 1, 2, 3, \dots$

For the orbital angular momentum $\widehat{\mathbf{L}} = \widehat{\mathbf{r}} \wedge \widehat{\mathbf{p}}$. In the coordinate representation $\widehat{\mathbf{r}} = \mathbf{r}$ and $\widehat{\mathbf{p}} = -i\nabla_{\mathbf{r}}$. From the commutation relations for position and momentum

$$[\widehat{r}_i, \widehat{r}_j] = 0, \quad (\text{B13})$$

$$[\widehat{p}_i, \widehat{p}_j] = 0, \quad (\text{B14})$$

$$[\widehat{r}_i, \widehat{p}_j] = i\delta_{ij}, \quad (\text{B15})$$

follows

$$[\widehat{L}_i, \widehat{r}_j] = i\epsilon_{ijk}\widehat{r}_k, \quad (\text{B16})$$

$$[\widehat{L}_i, \widehat{p}_j] = i\epsilon_{ijk}\widehat{p}_k, \quad (\text{B17})$$

and again Eq. (B1). Using spherical coordinates

$$r_1 = r \sin \theta \cos \phi, \quad r_2 = r \sin \theta \sin \phi, \quad r_3 = r \cos \theta, \quad (\text{B18})$$

we find in particular

$$\widehat{L}_3 = -i \frac{\partial}{\partial \phi}. \quad (\text{B19})$$

So we see that the eigenvalue equation

$$\widehat{L}_3\psi_{L,M}(\mathbf{r}) = M\psi_{L,M}(\mathbf{r}), \quad (\text{B20})$$

has solution

$$\psi_{L,M} = f(r, \theta)e^{iM\phi}, \quad (\text{B21})$$

where f is an arbitrary function. If the function $\psi_{L,M}$ has to be single valued, it must be periodic in ϕ with period 2π . Hence we find that additionally for the orbital case we must have $M = 0, \pm 1, \pm 2, \dots$, i.e. L must be an integer.

If we have to add the angular momentum of two different systems, $\widehat{L} = \widehat{L}^{(1)} + \widehat{L}^{(2)}$, we can either choose the set of commuting operators $\{(\widehat{L}^{(1)})^2, (\widehat{L}^{(2)})^2, \widehat{L}^{(1)}_3, \widehat{L}^{(2)}_3\}$ or the other one $\{(\widehat{L}^{(1)})^2, (\widehat{L}^{(2)})^2, \widehat{L}^2, \widehat{L}_3\}$, since $[\widehat{L}^{(1)}, \widehat{L}^{(2)}] = 0$.

AUTHOR DECLARATIONS

Conflicts of interest

None declared.

Data availability

The data that support the findings of this study are available from the corresponding author upon reasonable request.

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