

# Statistical Physics

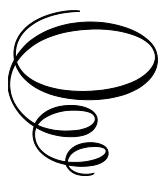


# Statistical Physics

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**Cambridge  
Scholars  
Publishing**



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This book first published 2021

Cambridge Scholars Publishing

Lady Stephenson Library, Newcastle upon Tyne, NE6 2PA, UK

British Library Cataloguing in Publication Data

A catalogue record for this book is available from the British Library

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ISBN (10): 1-5275-7449-0

ISBN (13): 978-1-5275-7449-6

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# 1 Preface

Let us consider an ideal classical gas consisting of  $N$  identical molecules (atoms) in a container with volume  $V$ ; the molecules are free of interaction (ideal gas) and obey the classical laws of Mechanics (classical gas). Each molecule collides with the walls of the container and suffers a change of momentum  $2mv_x$  along the  $x$ -direction, in an elastic collision, where  $m$  is the molecule mass and  $v_x$  is the  $x$ -component of the molecule velocity. Consequently, a force  $2mv_x/\Delta t$  is exerted upon the wall in the collision duration  $\Delta t$ . During this time  $\frac{1}{2}nv_x\Delta t\Delta S$  molecules hit the area element  $\Delta S$  of the wall, with the same velocity, where  $n$  is the density of molecules. We note that  $n$  is a function of position, and we associate a molecular velocity to that position. This amounts to a continuum model of the gas. The total force exerted on  $\Delta S$  is  $2mv_x/\Delta t \cdot \frac{1}{2}nv_x\Delta t\Delta S = nmv_x^2\Delta S$ . Therefore, a pressure  $p = nmv_x^2$  is exerted on  $\Delta S$  during this molecular collision. The molecular velocities are different for various collisions occurring in various moments of time, such that it is reasonable to take a mean value  $\overline{v_x^2} = \frac{1}{3}\overline{v^2}$  and a pressure  $p = \frac{1}{3}nm\overline{v^2} = \frac{2}{3}n\overline{w}$ , where  $\overline{w}$  is the mean energy of a molecule. Noteworthy, the velocities and their components are viewed as independent statistical quantities. Obviously, this pressure may generate a change

$$dE = -pdV \tag{1.1}$$

in the energy of the gas. It is worth noting that this result (the pressure) is not derived from the mechanical laws of molecular motion. The additional element in this derivation is the mean value of the energy, which implies a statistical distribution. We say that the gas is a statistical ensemble.

A statistical distribution should have a probability density  $\rho$  and a statistical set of variables. The molecular collisions may occur for various momenta  $\mathbf{p}$  and positions  $\mathbf{r}$  of a molecule. It is worth noting

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that  $\mathbf{p}$  and  $\mathbf{r}$  are not related by a mechanical trajectory. Therefore, we may view the mechanical states labelled by the set of momenta ( $p$ ) and the set of positions ( $q$ ) as independent statistical variables. We denote by  $d\gamma$  the element of the number of states for one molecule, and by  $d\Gamma$  the element of the number of states for the whole gas. We can write

$$\overline{w} = \int \rho w d\gamma . \quad (1.2)$$

A mean-value theorem shows  $\overline{w} = \overline{w}\rho\gamma$ , *i.e.*  $\rho = 1/\gamma$  and  $d\overline{w} = \overline{w}d(\ln \gamma)$ . It is convenient to denote  $\overline{w} = \frac{3}{2}T$  and  $\ln \gamma = f$ ,  $\overline{\ln \gamma} = \overline{f} = s$ ; it follows  $d\overline{w} = Tds$  and

$$dE = TdS \quad (1.3)$$

for the whole gas. We call the parameter  $T$  temperature and  $f$ ,  $\overline{f}$  the entropy of a molecule,  $\mathcal{S} = Nf$ ,  $S = Ns$  the entropy of the gas. Indeed, the number of states is multiplicative with respect to the number of molecules, such that its logarithm is additive. The change in energy is

$$dE = -pdV + TdS . \quad (1.4)$$

We can see that this change of energy has nothing to do with the mechanical motion.  $dQ = TdS$  is called heat. Indeed, the change of mechanical energy is

$$\begin{aligned} dE &= \frac{\partial E}{\partial q_i} dq_i + \frac{\partial E}{\partial p_i} dp_i = \frac{\partial E}{\partial q_i} \dot{q}_i dt + \frac{\partial E}{\partial p_i} \dot{p}_i dt = \\ &= \frac{\partial E}{\partial q_i} \frac{\partial E}{\partial p_i} dt - \frac{\partial E}{\partial p_i} \frac{\partial E}{\partial q_i} dt = 0 , \end{aligned} \quad (1.5)$$

*i.e.* the energy is conserved in mechanical motion.

From  $\rho = 1/\Gamma$  and  $\mathcal{S} = \ln \Gamma$  we get  $\rho = e^{-\mathcal{S}}$ . Since the mean energy is minimal for an isolated ensemble, the statistical distribution  $\rho$  should be minimal, so the entropy should be maximal. A minimal  $\rho$  means a molecular chaos. The isolated ensembles evolve towards the maximum of the entropy, where the disorder is maximal. This is the law of increase of entropy. In addition, when the molecular motion ceases, the temperature is zero and the ensemble occupies one state; therefore, at zero temperature the entropy is zero. An isolated ensemble has the tendency to increase its volume (in order to minimize the energy).

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From equation (1.4) we get  $d(E - TS) = -pdV - SdT$ , where  $F = E - TS$ , called free energy, is the energy in variables  $V$  and  $T$ . Therefore, an isolated ensemble tends to increase the volume and to decrease the temperature. Free bodies get colder and the universe evolves towards its Waermetod.

The introduction of the mechanical states as statistical variables opens the way to a statistical description for quantum-mechanical ensembles as well, by replacing the integration over the number of mechanical states by summations over quantum-mechanical states. A quantum gas has an occupation number for each particle state. While the states are fixed, the occupation number may vary, such that the number of particles may vary. Indeed, from equation (1.4) we get

$$\begin{aligned} d(E + pV - TS) &= Vdp - SdT = \\ &= N(vdp - sdT) = Nd\mu \ , \end{aligned} \tag{1.6}$$

where  $v$  and  $s$  are the volume and the entropy per particle. It follows that the number of particles is variable, and

$$dE = -pdV + TdS + \mu dN \ , \tag{1.7}$$

such that  $d(E + pV - TS) = Nd\mu + \mu dN = d(\mu N)$ . The chemical potential  $\mu$  serves to fix the mean number of particles  $N$ . The probability density  $\rho$  is a function of  $\mathcal{S}$ , which should be a function of the energy  $\mathcal{E}$ , the volume  $V$  and the number of particles  $\mathcal{N}$  ( $N = \overline{\mathcal{N}}$ ); we may take as variables  $V$ ,  $\mathcal{N}$  and  $T$  instead of energy. To the first approximation the probability density can be written as  $\rho \sim e^{-(\partial\mathcal{S}/\partial\mathcal{E})(\mathcal{E} + \mu\mathcal{N})}$ , where  $(\partial\mathcal{S}/\partial\mathcal{E}) = 1/T$ . Possible configurational correlations may introduce a dependence on  $V$ . The approximation consists in neglecting deviations from mean values, *i.e.* the fluctuations. For independent statistical variables the fluctuations go like  $\overline{\Delta f^2} = \sum_{ij} \overline{\Delta f_i \Delta f_j} \sim N$ ; therefore, the approximation is valid in the limit of large  $N$  ( $N \gg 1$ ). We can see that the statistical description, which arises from an ideal classical gas, can be applied to many other ensembles, of a reasonable generality.



## 2 Introduction

### 2.1 Mechanics

At first sight the space is homogeneous and isotropic and the time flows uniformly. A body, viewed as a point, covers a small distance  $\Delta \mathbf{r}$  in the small duration  $\Delta t$ , where  $\mathbf{r}$  is its position at time  $t$ . Since the space and the time are uniform, in the next time interval  $\Delta t$  the point covers the same distance  $\Delta \mathbf{r}$ , with the same magnitude and the same direction as the previous one. The small quantities  $\Delta \mathbf{r}$  and  $\Delta t$  may vary, but each time their ratio  $\Delta \mathbf{r}/\Delta t$  is the same. In order to eliminate the arbitrary variation of  $\Delta \mathbf{r}$  and  $\Delta t$  we take both  $\Delta \mathbf{r}$  and  $\Delta t$  simultaneously to zero, *i.e.* they are so small that we may neglect them. It follows that the motion is such that the velocity

$$\mathbf{v} = \lim_{\Delta t \rightarrow 0} \frac{\Delta \mathbf{r}}{\Delta t} = \frac{d\mathbf{r}}{dt} \quad (2.1)$$

is a constant. This is Newton's Principle of Inertia. The position of the point is modified during the time, but its velocity is constant. This law identifies the velocity as the basic quantity which describes the motion. If the space, or the time, or both are not uniform, then the velocity changes in time. According to the notation introduced in equation (2.1) this change is written as  $d\mathbf{v}/dt$ . It is caused by a property of the space and the time, the presence of other bodies; we call it force, denoted by  $\mathbf{F}$ . The change may also depend on the properties of the moving body; we call this property the mass of the body, denoted by  $m$ . This is an unknown quantity. The law of the change of the velocity can therefore be written as

$$m \frac{d\mathbf{v}}{dt} = \mathbf{F} . \quad (2.2)$$

This is Newton's law of motion, known also as  $\mathbf{F} = m\mathbf{a}$ , where  $\mathbf{a} = d\mathbf{v}/dt$  is called acceleration. It is worth noting that, although

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the bodies are viewed in Mechanics as being point-like (or consisting of point-like bodies), the motion is made by infinitesimal distances and durations, not by points. This special contradiction permeates the whole Physics and calls for a special caution. If we give the position and the velocity at one point, then the motion is determined at the subsequent point. It follows that the equation (2.2) written as  $m d^2 \mathbf{r} / dt^2 = \mathbf{F}$  should be a second-order differential equation, *i.e.* the ratio  $\mathbf{F}/m$  should be a function of time, position and velocity at most; this equation gives the trajectory of the motion.

The Newton law of motion can be solved for a body in an external force field and for two interacting bodies; for more than two bodies it has, practically, no solution. This is an imperfection of the theory.

## 2.2 Electromagnetism

Let point-like electrical charges  $q$  be distributed in space with a uniform concentration  $n$ ; and let a rigid neutralizing background of charges  $-q$  be also present. The electrical charge  $q$  is an unknown quantity. Let  $\mathbf{u}$  be a local displacement; it produces a net charge density  $\rho = -nq \operatorname{div} \mathbf{u}$ . Let us call  $-4\pi nq \mathbf{u}$  electric field, denoted by  $\mathbf{E}$ . It follows

$$\operatorname{div} \mathbf{E} = 4\pi \rho . \quad (2.3)$$

This is the Gauss law of the electric field and the first Maxwell equation.

By introducing fields, like the displacement  $\mathbf{u}$  and the electric field  $\mathbf{E}$ , the Electromagnetism departs from Mechanics. When mechanical point-like charges are used, with density of the form  $\rho = q\delta(\mathbf{r})$ , singular solutions are obtained, like  $\mathbf{E} = q\mathbf{r}/r^3$  (Coulomb law). This contradictory framework calls for certain limitations.

We note that  $\mathbf{p} = q\mathbf{u}$  is a dipole moment;  $\mathbf{P} = n\mathbf{p}$  is a density of dipole moments, called polarization (and, here,  $\mathbf{E} = -4\pi\mathbf{P} = -4\pi n\mathbf{p}$ ).

There exists a similar quantity. Indeed, apart from a displacement  $\mathbf{u}$ , a charge  $q$  with position  $\mathbf{r}_a$  may rotate about a point placed at  $\mathbf{r}$  with velocity  $\mathbf{v}_a$ . The quantity  $q\mathbf{v}_a$  is a current,  $\mathbf{j}_m = nq\mathbf{v}_a$  is a current density, and the quantity  $(\mathbf{r}_a - \mathbf{r}) \times q\mathbf{v}_a$  would be similar to  $\mathbf{p}$ , provided we divide it by a velocity  $c$ .

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It is worth noting that the velocity  $c$  is a universal velocity, independent of the charges, or the space, time, etc. It is an unknown quantity.

We call  $\mathbf{m} = (\mathbf{r}_a - \mathbf{r}) \times q\mathbf{v}_a/2c$  magnetic moment, and  $\mathbf{M} = (\mathbf{r}_a - \mathbf{r}) \times \mathbf{j}_m/2c$  magnetization. For small magnitudes of the rotation radius  $\mathbf{r}_a - \mathbf{r}$  the magnetic moments are a distinct type of moments of point-like charges. The magnetization has the remarkable property  $\text{curl}\mathbf{M} = \mathbf{j}_m/c$ . Let us call  $\mathbf{B} = 4\pi\mathbf{M} = 4\pi n\mathbf{m}$  magnetic induction. It satisfies the equation

$$\text{curl}\mathbf{B} = \frac{4\pi}{c}\mathbf{j}_m = 4\pi\text{curl}\mathbf{M} . \quad (2.4)$$

The magnetization current has the property  $\text{div}\mathbf{j}_m = 0$ . But there exists another current, corresponding to the displacement  $\mathbf{u}$ , given by  $\mathbf{j} = nq\dot{\mathbf{u}}$ . Therefore, the above equation should be written as

$$\text{curl}\mathbf{B} = \frac{4\pi}{c}\mathbf{j} + 4\pi\text{curl}\mathbf{M} , \quad (2.5)$$

or, denoting  $\mathbf{H} = \mathbf{B} - 4\pi\mathbf{M}$ ,

$$\text{curl}\mathbf{H} = \frac{4\pi}{c}\mathbf{j} ; \quad (2.6)$$

$\mathbf{H}$  is called magnetic field. Equation (2.6) is the Ampere equation and, partially, the fourth Maxwell equation. At this moment there appears a contradiction between equations (2.3) and (2.6). Indeed, by the continuity equation, we get from equation (2.3)  $\text{div}\dot{\mathbf{E}} = 4\pi\dot{\rho} = -4\pi\text{div}\mathbf{j}$ , while  $\text{div}\mathbf{j} = 0$  from equation (2.6). The contradiction disappears if we add the term  $\dot{\mathbf{E}}/c$  to the right of equation (2.6), which reads now

$$\text{curl}\mathbf{H} = \frac{1}{c}\frac{\partial\mathbf{E}}{\partial t} + \frac{4\pi}{c}\mathbf{j} . \quad (2.7)$$

This is Maxwell-Ampere equation and the fourth Maxwell equation. Again, a constant point-like current  $I$  leads to  $\Delta\mathbf{A} = -\frac{4\pi}{c}\mathbf{I}\delta(\mathbf{r})$ , where  $\mathbf{H} = \text{curl}\mathbf{A}$ ,  $\text{div}\mathbf{A} = 0$ , and  $\mathbf{H} = \frac{1}{c}\mathbf{I} \times \mathbf{r}/r^3$  (Biot-Savart law), which is singular in origin.

Moreover, from the definition  $\mathbf{m} = (\mathbf{r}_a - \mathbf{r}) \times q\mathbf{v}_a/2c$  it follows  $\text{div}\mathbf{m} = 0$ ,  $\text{div}\mathbf{M} = 0$  and

$$\text{div}\mathbf{B} = 0 . \quad (2.8)$$

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This is the Gauss equation for the magnetic induction and the second Maxwell equation. It shows that there is no magnetic charge.

We note that, if the charges belong to a material medium, this medium disappears from equations (2.3) and (2.7), so we may view these equations as valid for vacuum; or an immaterial medium, which historically is called aether. In vacuum  $\mathbf{B} = \mathbf{H}$  and equation (2.8) reads

$$\text{div} \mathbf{H} = 0 . \quad (2.9)$$

Finally, we note that there exists a symmetry between  $\mathbf{E}$  and  $\mathbf{B}$ , since both are given by moments of charges ( $\mathbf{p}$  and  $\mathbf{m}$ ). It is worth noting that while  $\mathbf{E}$  is related to  $-4\pi n\mathbf{p}$ , the magnetic induction is related to  $4\pi n\mathbf{m}$ . Therefore, in writing down this symmetry we should note that  $\mathbf{E}$  corresponds to  $-\mathbf{B}$  and there is no magnetic charge and no associated current. Equation (2.7) reads

$$\text{curl} \mathbf{B} = \frac{1}{c} \frac{\partial \mathbf{E}}{\partial t} + \frac{4\pi}{c} \mathbf{j} + 4\pi \text{curl} \mathbf{M} \quad (2.10)$$

for the couple  $\mathbf{B}, \mathbf{E}$ ; therefore, the corresponding equation for the couple  $\mathbf{E}, \mathbf{B}$  reads

$$\text{curl} \mathbf{E} = -\frac{1}{c} \frac{\partial \mathbf{B}}{\partial t} . \quad (2.11)$$

This is the Faraday equation and the third Maxwell equation. In vacuum it reads  $\text{curl} \mathbf{E} = -\frac{1}{c} \frac{\partial \mathbf{H}}{\partial t}$ .

The Faraday equation can be derived in another way. According to the Helmholtz theorem the variation of the displacement  $\mathbf{u}$  is given by

$$du_i = \partial_j u_i dx_j = \frac{1}{2} (\partial_j u_i + \partial_i u_j) dx_j + \frac{1}{2} (\partial_j u_i - \partial_i u_j) dx_j . \quad (2.12)$$

The first bracket in equation (2.12) indicates a deformation, *i.e.* a change in the element of the distance  $dl = (dx_i^2)^{1/2}$ . The second bracket indicates a rotation; indeed, it can be written as

$$du_i^{\text{rot}} = \frac{1}{2} (\partial_j u_i - \partial_i u_j) dx_j = \frac{1}{2} (\text{curl} \mathbf{u} \times d\mathbf{r})_i , \quad (2.13)$$

or

$$d\mathbf{u}^{\text{rot}} = \frac{1}{2} \text{curl} \mathbf{u} \times d\mathbf{r} ; \quad (2.14)$$



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we can see that  $\text{curl}\mathbf{u}$  is a rotation angle  $\varphi$ . It follows that  $d\mathbf{u}^{rot}$  is related to the rotation connected to the magnetic moment, such that the electric field is related to the magnetic induction. Indeed, from equation (2.14) we get

$$\text{curl}\mathbf{u} = \frac{2}{dr^2}d\mathbf{r} \times d\mathbf{u}^{rot} , \quad (2.15)$$

which can be written as

$$\begin{aligned} \text{curl}\mathbf{u} &= \frac{2dt}{dr^2}d(\mathbf{r}_a - \mathbf{r}) \times \mathbf{v}_a = \frac{4cdt}{nqdr^2}d(\mathbf{r}_a - \mathbf{r}) \times \mathbf{j}_m/2c = \\ &= \frac{cdt}{\pi nqdr^2}d\mathbf{B} . \end{aligned} \quad (2.16)$$

In this equation  $d\mathbf{r} = d(\mathbf{r}_a - \mathbf{r})$ ; the variation of this quantity may be set equal to  $2cdt$ , such that we get

$$\text{curl}\mathbf{u} = \frac{1}{4\pi nqcdt}d\mathbf{B} , \quad (2.17)$$

or

$$\text{curl}\mathbf{E} = -\frac{1}{c}\frac{\partial\mathbf{B}}{\partial t} . \quad (2.18)$$

It is worth noting that equations  $\text{div}\mathbf{E} = 4\pi\rho$  and  $\text{div}\mathbf{H} = 0$  (in vacuum) follow from equations

$$\begin{aligned} \text{curl}\mathbf{H} &= \frac{1}{c}\frac{\partial\mathbf{E}}{\partial t} + \frac{4\pi}{c}\mathbf{j} , \\ \text{curl}\mathbf{E} &= -\frac{1}{c}\frac{\partial\mathbf{H}}{\partial t} \end{aligned} \quad (2.19)$$

and the continuity equation. It follows that only two (coupled) Maxwell equations are independent, which include two unknown vectors  $\mathbf{E}$  and  $\mathbf{H}$  (or, similarly,  $\mathbf{E}$  and  $\mathbf{B}$ , provided  $\mathbf{M}$  is known). This means that we have in fact only one unknown field vector.

As it is well known the standard way of solving the Maxwell equations is the introduction of the scalar potential  $\Phi$  and the vector potential  $\mathbf{A}$  through

$$\mathbf{E} = -\frac{1}{c}\frac{\partial\mathbf{A}}{\partial t} - \text{grad}\Phi , \quad \mathbf{B} = \text{curl}\mathbf{A} , \quad (2.20)$$

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assuming  $\mathbf{M}$  is known. In vacuum  $\mathbf{B} = \mathbf{H}$  and we get the wave equations

$$\frac{1}{c^2} \frac{\partial^2 \mathbf{A}}{\partial t^2} - \Delta \mathbf{A} = \frac{4\pi}{c} \mathbf{j} , \quad \frac{1}{c^2} \frac{\partial^2 \Phi}{\partial t^2} - \Delta \Phi = 4\pi \rho , \quad (2.21)$$

providing the Lorenz gauge

$$\frac{1}{c} \frac{\partial \Phi}{\partial t} + \text{div} \mathbf{A} = 0 \quad (2.22)$$

is satisfied; this condition reduces the number of four unknowns of the potentials to three. The wave equations have also advanced solutions, which are unphysical; they are discarded. These solutions originate in the existence of the velocity  $c$  and are an imperfection of the theory.

The electrical charge is extraneous to the theory of electromagnetism. Similarly, the universal velocity  $c$  introduced in the definition of the magnetic moment, the magnetic induction and the magnetic field is arbitrary. Not only "the electrical charge is a stranger" in Electromagnetism (Einstein, Pauli), but also the universal velocity  $c$  is a stranger. The velocity  $c$  of the electromagnetic waves has been measured. It coincides with the measured speed of light,  $c = 3 \times 10^{10} \text{ cm/s}$ . This made Maxwell to suggest that light and electromagnetic radiation are the same thing.

The solution of the wave equations (2.21) is given by the Kirchhoff's (retarded) law

$$\Phi = \int d\mathbf{r}' \frac{\rho(\mathbf{r}', t - |\mathbf{r} - \mathbf{r}'|)}{|\mathbf{r} - \mathbf{r}'|} \quad (2.23)$$

(for the scalar potential); For  $\rho = q\delta(\mathbf{r})f(t)$  we get  $\Phi = qf(t - r/c)/r$ , which, apart from being propagated, it is again singular at the origin.

In vacuum the Maxwell equations are

$$\begin{aligned} \text{div} \mathbf{E} &= 4\pi \rho , \quad \text{div} \mathbf{H} = 0 , \\ \text{curl} \mathbf{E} &= -\frac{1}{c} \frac{\partial \mathbf{H}}{\partial t} , \quad \text{curl} \mathbf{H} = \frac{1}{c} \frac{\partial \mathbf{E}}{\partial t} + \frac{4\pi}{c} \mathbf{j} . \end{aligned} \quad (2.24)$$

A polarization  $\mathbf{P} = nq\mathbf{u}$  appears in matter, from a charge density  $-nq\text{div} \mathbf{u} = -\text{div} \mathbf{P}$ ; it carries a current density  $\dot{\mathbf{P}}$ . In addition a magnetization  $\mathbf{M}$  may appear, from a magnetization current  $c \cdot \text{curl} \mathbf{M}$ ,

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and a magnetic induction  $\mathbf{B}$ . According to the above discussion, the Maxwell equations read

$$\begin{aligned} \operatorname{div} \mathbf{E} &= 4\pi\rho - 4\pi\operatorname{div} \mathbf{P} , \quad \operatorname{div} \mathbf{B} = 0 , \\ \operatorname{curl} \mathbf{E} &= -\frac{1}{c} \frac{\partial \mathbf{B}}{\partial t} , \end{aligned} \tag{2.25}$$

$$\operatorname{curl} \mathbf{B} = \frac{1}{c} \frac{\partial \mathbf{E}}{\partial t} + \frac{4\pi}{c} \dot{\mathbf{P}} + \frac{4\pi}{c} \mathbf{j} + 4\pi\operatorname{curl} \mathbf{M} ,$$

or, introducing the electric displacement (induction)  $\mathbf{D} = \mathbf{E} + 4\pi\mathbf{P}$  and using the magnetic field  $\mathbf{H} = \mathbf{B} - 4\pi\mathbf{M}$ ,

$$\begin{aligned} \operatorname{div} \mathbf{D} &= 4\pi\rho , \quad \operatorname{div} \mathbf{B} = 0 , \\ \operatorname{curl} \mathbf{E} &= -\frac{1}{c} \frac{\partial \mathbf{B}}{\partial t} , \quad \operatorname{curl} \mathbf{H} = \frac{1}{c} \frac{\partial \mathbf{D}}{\partial t} + \frac{4\pi}{c} \mathbf{j} . \end{aligned} \tag{2.26}$$

Again, only the two equations (2.26) in the second row are independent, but now they include four unknown vectors. Additional information is necessary to reduce the number of these unknowns to two.

The displacement  $\mathbf{u}$  obeys the equation of motion

$$m\ddot{\mathbf{u}} + m\omega_c^2\mathbf{u} + m\gamma\dot{\mathbf{u}} = q\mathbf{E}_0 + q\mathbf{E}_i \tag{2.27}$$

for a charge  $q$  with mass  $m$  in an external electric field  $\mathbf{E}_0$ , where  $\omega_c$  is a characteristic frequency,  $\gamma$  is a dissipation coefficient and  $\mathbf{E}_i = -4\pi nq\mathbf{u}$  is the internal (polarization) electric field. This equation allows the definition of a polarizability  $\alpha$  by  $\mathbf{P} = \alpha\mathbf{E}_0$  and the definition of the electrical susceptibility  $\chi_e$  by  $\mathbf{P} = \chi_e\mathbf{E}_t$ , where  $\mathbf{E}_t = \mathbf{E}_0 + \mathbf{E}_i = \mathbf{E}$ , as well as the definition of the dielectric function  $\varepsilon$  by  $\mathbf{E}_0 = \varepsilon\mathbf{E}_t$ ; the external field  $\mathbf{E}_0$  turns out to be the electric displacement  $\mathbf{D}$ . The polarizability may include also the atomic and molecular polarizability, the molecular vibrational polarizability, the molecular rotational polarizability and the Curie-Langevin orientational polarizability of the electric moments, proportional to the inverse of the temperature  $1/T$ . These relations establish a connection between  $\mathbf{D}$  and  $\mathbf{E}$ .

Similarly, the equation of motion of the magnetization is  $\dot{\mathbf{M}} = \frac{q}{2mc} \mathbf{M} \times \mathbf{B}$ , or  $\dot{\mathbf{M}} = \gamma \mathbf{B} \times \mathbf{M}$ , where  $\gamma = \mu/\hbar$  is the gyromagnetic factor and  $\mu$  is the magnetic moment. This equation does not establish a relation

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between  $\mathbf{M}$  and  $\mathbf{B}$ , but it indicates an eigenfrequency of the magnetization, given by the magnetic induction. The magnetic susceptibility  $\chi_m$  defined by  $\mathbf{M} = \chi_m \mathbf{H}$  and the magnetic permeability defined by  $\mathbf{B} = \mu \mathbf{H}$  are derived by the induced magnetic moment in an external magnetic field (diamagnetic susceptibility) and the alignment of the statistical magnetic moments (Curie-Langevin law).

## 2.3 Relativity

The universal velocity  $c$  which appears in the Maxwell equations has far-reaching implications. First, we should note that in the time variation written as  $\frac{d}{dt} = \frac{\partial}{\partial t} + \mathbf{v} \frac{\partial}{\partial \mathbf{r}}$  we may view  $t$  and  $\mathbf{r}$  as independent variables, but we may also view  $t$  and  $\mathbf{r}$  as being related through the velocity  $\mathbf{v}$ . Second, the electromagnetic waves propagate such as  $c dt - d\mathbf{l} = 0$  (retarded waves), where  $d\mathbf{l}$  is the infinitesimal distance, but they propagate also as  $c dt + d\mathbf{l} = 0$  (advanced waves), which is unphysical. Therefore, we must admit the relation  $c^2 dt^2 - d\mathbf{l}^2 = 0$  for electromagnetic waves, or  $c^2 dt^2 - d\mathbf{r}^2 = 0$ . This means that we may change the reference frame by a constant velocity  $\mathbf{v}$  and this relation is preserved. For bodies moving with velocity  $\mathbf{v}$  this relation should read  $c^2 dt^2 - v^2 dt^2 = c^2 d\tau^2 > 0$ , where  $\tau$  is the time measured at rest (proper time). It follows that  $c$  is the maximum velocity in the universe. Also, it follows that the change of coordinates in referential frames, *i.e.* frames moving with constant velocities with respect to each other, should obey the condition  $c^2 dt^2 - d\mathbf{r}^2 = ds^2 = \text{const}$ ;  $ds$  is called the element of the line of universe. The coordinate transformations which preserve this condition are the Lorentz transformations. Moreover, the Maxwell equations preserve their form under these transformations, such that the relativity principle for electromagnetic waves is satisfied. This can be seen very easily by using four-vector notations: contravariant vectors like  $x^\mu = (ct, \mathbf{r})$  and covariant vectors like  $x_\mu = g_{\mu\nu} x^\nu$ , where  $g_{00} = 1$ ,  $g_{11} = g_{22} = g_{33} = -1$ , otherwise zero. Similarly, the electromagnetic potentials are  $A^\mu = (\Phi, \mathbf{A})$ , the field tensor is  $F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu$  and the Maxwell equations

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become

$$\begin{aligned}\partial_\rho F_{\mu\nu} + \partial_\mu F_{\nu\rho} + \partial_\nu F_{\rho\mu} &= 0 , \\ \partial_\nu F^{\mu\nu} &= -\frac{4\pi}{c} j^\mu ,\end{aligned}\tag{2.28}$$

with the Lorentz condition  $\partial_\mu A^\mu = 0$ , where  $j^\mu = (c\rho, \mathbf{j})$  is the current density (and  $\partial_\mu = \partial/\partial x^\mu$ ). The equations for the potentials are  $\partial_\nu \partial^\nu A^\mu - \partial^\mu (\partial_\nu A^\nu) = \frac{4\pi}{c} j^\mu$ .

On the other hand, the Fermat (or Maupertuis') principle for a moving body with mass  $m$  is immediately generalized to the extremum of the action

$$S = -mc \int ds = -mc^2 \int \sqrt{1 - v^2/c^2} dt ,\tag{2.29}$$

which leads to the lagrangian

$$L = -mc^2 \sqrt{1 - v^2/c^2} ,\tag{2.30}$$

the momentum

$$\mathbf{p} = \frac{\partial L}{\partial \mathbf{v}} = \frac{m\mathbf{v}}{\sqrt{1 - v^2/c^2}}\tag{2.31}$$

and the energy

$$\mathcal{E} = \mathbf{v}\mathbf{p} - L = \frac{mc^2}{\sqrt{1 - v^2/c^2}} = mc^2 + \frac{1}{2}mv^2 + \dots ,\tag{2.32}$$

whence we can see the rest energy  $mc^2$ . In addition,  $\mathcal{E}^2 = m^2 c^4 + p^2 c^2$  and  $\mathcal{E}d\mathcal{E} = c^2 \mathbf{p}d\mathbf{p}$ ,  $d\mathcal{E} = \mathbf{v}d\mathbf{p}$ . The variation of the action gives

$$\delta S = -mcu_\mu \delta x^\mu + mc \int \delta x^\mu \frac{du_\mu}{ds} ds ,\tag{2.33}$$

where

$$u^\mu = \frac{dx^\mu}{ds} = \left( \frac{1}{\sqrt{1 - v^2/c^2}}, \frac{\mathbf{v}}{c\sqrt{1 - v^2/c^2}} \right)\tag{2.34}$$

is the four-dimensional velocity. Also, from equation (2.33), the four-dimensional momentum is

$$p_\mu = -\frac{\delta S}{\delta x^\mu} = mcu_\mu ,\tag{2.35}$$

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or

$$p^\mu = mcu^\mu = \left( \frac{mc}{\sqrt{1-v^2/c^2}}, \frac{m\mathbf{v}}{\sqrt{1-v^2/c^2}} \right) = (\mathcal{E}/c, \mathbf{p}) \quad (2.36)$$

(and  $p^\mu p_\mu = m^2 c^2$ ). The variation of the action in equation (2.33) gives also the equations of motion

$$\begin{aligned} \frac{dp^\mu}{ds} &= \frac{1}{c\sqrt{1-v^2/c^2}} \left( \frac{1}{c} \frac{d\mathcal{E}}{dt}, \frac{d\mathbf{p}}{dt} \right) = \\ &= \frac{1}{c\sqrt{1-v^2/c^2}} \left( \frac{1}{c} \frac{v d\mathbf{p}}{dt}, \frac{d\mathbf{p}}{dt} \right) = \\ &= \frac{1}{c\sqrt{1-v^2/c^2}} \left( \frac{1}{c} \mathbf{v} \mathbf{f}, \mathbf{f} \right) = g^\mu, \end{aligned} \quad (2.37)$$

where  $g^\mu$  is the generalization of the force  $\mathbf{f}$ ; or  $d\mathcal{E}/dt = \mathbf{v} \mathbf{f}$  and  $d\mathbf{p}/dt = \mathbf{f}$ . This way, the motion of the bodies satisfies the relativity principle. Therefore, the relativity principle is satisfied by both the electromagnetic equations and the mechanical equations; extended to all motions it is called Einstein's Principle of Relativity. The specific way it works is called the Theory of Relativity. We note that, although the electromagnetic equations indicate the necessity of Lorentz transformations for coordinates, this requirement for other vectors, tensors follows from the Principle of Relativity.

As it is well known the Maxwell equations in vacuum lead to the Lorentz force  $\rho \mathbf{E} + \frac{1}{c} \mathbf{j} \times \mathbf{H}$  which acts upon charges and currents. Making use of  $\mathbf{j}_\mu = \rho \mathbf{u}_\mu \frac{ds}{dt}$  and the field tensor  $F^{\mu\nu}$  defined above this force density can be written as  $\frac{1}{c} \rho F^{\mu\nu} u_\nu$ , such that the equation of motion for the mass density  $\mu$  is

$$\mu c \frac{du^\mu}{ds} = \frac{1}{c} \rho F^{\mu\nu} u_\nu. \quad (2.38)$$

We can see that the four-dimensional velocity determine the electromagnetic field through the Maxwell equations (2.28), and, conversely, the electromagnetic field determines the four-dimensional velocities through the equations of motion (2.38). Obviously, this is a self-interaction, which is unphysical. It should be avoided, by treating

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these equations separately, as if the charges, or the fields, were external. The estimation of the self-interaction effects leads to the Lorentz damping, which indicates the limits of such an improper formulation of the problem. In particular, such restrictions lead to distances larger than the classical charge radius  $e^2/mc^2$ , or Compton's wavelength  $\hbar/mc = (e^2/mc^2) \frac{\hbar c}{e^2}$ , where  $e$  is the charge,  $m$  is the particle mass,  $\hbar$  is Planck's constant and  $e^2/\hbar c = 1/137$  is the fine structure constant. Also, the fields should be restricted to Schwinger limit  $e/(e^2/mc^2)^2 = m^2 c^4/e^3$ , or  $mc^2/e(\hbar/mc) = (m^2 c^4/e^3) \frac{e^2}{\hbar c}$ , which is a very high field. If  $e$  is the electron charge ( $e = 4.8 \times 10^{10} esu$ ) and  $m$  is the electron mass ( $m = 10^{-27} g$ ), the rest energy of the electron is  $mc^2 = 0.5 MeV$  ( $1eV = 1.6 \times 10^{-12} erg$ ), the classical electron radius is  $r_e = e^2/mc^2 = 2.8 \times 10^{-13} cm$ , the Compton wavelength of the electron is  $\lambda_e = \hbar/mc = 3.8 \times 10^{-11} cm$  and Schwinger's limit for the fields is  $E_s = mc^2/e(\hbar/mc) = 6 \times 10^{13} esu$  ( $1esu = 3 \times 10^4 V/m$ ). Beyond these limits the Electromagnetism, either classical or quantum-mechanical, becomes meaningless.

## 2.4 Quantum Mechanics

The world is made of many small, very small, particles, which we call atoms and molecules; which may have their own structure, consisting of subatomic particles, like the electron, the proton, the neutron, etc. Of course, such particles are much more numerous than the big bodies, *i.e.* bodies with dimensions at the macroscopic scale. Mainly the atomic particles move over limited small spatial regions, such that it may not only be impossible to fully characterize their motion, but, often, not even desirable. An example is the small magnetic moments which served above to define the magnetic field. We may expect a certain indefiniteness, a certain uncertainty in characterizing the motion of the atomic and subatomic particles; for instance, we may not expect to be possible to define a trajectory of such moving particles. Rather, we may speak of waves (actually oscillations), which would characterize a mechanical state. However, the motion over a limited spatial region can be describable globally by local differential equations; consequently, it has a certain characteristic imposed by boundary conditions, which implies discrete values of the physical quantities.

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Indeed, the conditions satisfied at a portion of the boundary, should meet the conditions satisfied at the opposite portion of the boundary. Of course, speaking in such terms we should have a wavefunction obeying certain differential equations, which defines mechanical states characterized by discrete values of the physical quantities.

Indeed, Planck realized that the electromagnetic radiation with frequency  $\omega$ , exchanged by the atoms of the wall of a black body, has energies which are integral multiples of  $\hbar\omega$ , where  $\hbar = 10^{-27} \text{erg} \cdot \text{s}$  is a universal constant, called Planck's constant. This is an unknown. Einstein gives individuality to this quantum of energy, which later was called photon. Rutherford suggested that the electrons moving about the nucleus in an atom have a discrete set  $E_n$  of energy levels, where  $n$  labels these levels. We arrive at speaking rather of a motion state for such particles, instead of definite mechanical quantities. An electromagnetic radiation with frequency  $\omega = 10^{15} \text{s}^{-1}$  would have an energy quantum  $\hbar\omega = 10^{-12} \text{erg}$ , which may be exchanged with the electrons in an atom. Being so small, how would we measure it? We will measure it only indirectly, by measuring many such identical processes. It follows that the measurement has a statistical character and, also, during the measurement the measured mechanical motion would be perturbed, to a smaller or a larger extent. We can see that the motion of these atomic and subatomic particles implies quanta of energy. We say that this motion is quantized. This is the Quantum-Mechanical Principle of motion. Quantum Mechanics introduces many new concepts for describing the motion, so it needs a longer discussion.

Motion is described by functions of time; any such function is decomposable in a Fourier series,

$$F(t) = \frac{1}{2\pi} \int d\omega e^{-i\omega t} F(\omega) ; \quad (2.39)$$

according to the quantization idea, we can replace  $\omega$  in this equation by  $\omega = E/\hbar$ , where  $\hbar = h/2\pi$ ,  $h$  and  $\hbar$  being Planck's constants. However, these energies are discrete, so we should have  $\omega_n = E_n/\hbar$ , where  $n$  is an integer, and the integral should be replaced by a summation. We measure only energy differences, such that we should have

$$e^{-\frac{i}{\hbar}(E_m - E_n)t} \quad (2.40)$$



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instead of  $e^{-i\omega t}$ , where  $n, m$  denote sets of integers; in this case  $F(\omega)$  should be replaced by a quantity denoted  $F_{nm}$ , such that

$$F(t) = \sum_{n,m} e^{-\frac{i}{\hbar}(E_m - E_n)t} F_{nm} ; \quad (2.41)$$

this was the starting point of Heisenberg's matricial mechanics. The representation given by equation (2.40) is a new representation for time-dependent functions, with far-reaching implications. We note the principle that "only measurable quantities are admitted in theory" (which, in fact, is a relative principle) and the additional freedom brought by two labels instead of one in equation (2.41).

The quantities  $F_{nm}$  were recognised to be matrix elements. This implies that an operator  $F$  is associated to any physical quantity.  $F$  acts in a linear space of vectors  $\varphi, \psi, \dots$  with a scalar product of the form  $(\varphi, \psi)$ ; the operator  $F$  has eigenvectors  $\varphi_n$  and eigenvalues  $f_n$ , such that

$$F\varphi_n = f_n\varphi_n ; \quad (2.42)$$

the matrix elements are written as

$$F_{nm} = (\varphi_n, F\varphi_m) , \quad (2.43)$$

and the mean value is  $F_{nn} = (\varphi_n, F\varphi_n)$ , or, generally,  $\overline{F} = (\varphi, F\varphi)$ . We may assume that the mean values are measurable quantities and the eigenvalue  $f_n$  is the value the quantity  $F$  has in the state  $\varphi_n$ ; since they are real, the associated operators should be self-adjoint (hermitian). A hermitian operator has orthogonal eigenvectors for distinct eigenvalues. If there exist several eigenvectors for the same eigenvalue, that eigenvalue is degenerate, and we can orthogonalize the degenerated eigenvectors; we may also orthonormalize the eigenvectors, *i.e.* we can impose the condition  $(\varphi_n, \varphi_m) = \delta_{nm}$ . The set of eigenvalues  $f_n$  is the spectrum of  $F$  (together with the corresponding eigenvectors); it may be discrete, or continuous; in the latter case the label  $n$  is continuous and we may write  $f_n$  as  $f(n)$  and summations of the type  $\sum_n$  should be replaced by  $\int dn$ ; the orthonormality condition reads in that case  $(\varphi_n, \varphi_m) = \delta(n - m)$ , where  $\delta$  is Dirac's delta function. By  $\sum$  or  $\int$  we understand indistinctly either  $\sum$ , or  $\int$ , or both.

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Since the eigenvectors are linearly independent (and orthogonal), they may be taken as a basis of expansion for any other vector

$$\psi = \sum_n c_n \varphi_n \quad , \quad (2.44)$$

where  $c_n$  are some complex coefficients. It follows that the vectors represent the states of the "physical system", and any state can be written as a superposition of other states; the operators act on the state vectors; the eigenvectors are also called eigenstates. This is the superposition principle of the Quantum Mechanics. The mean value is

$$\overline{F} = (\psi, F\psi) = \sum_n f_n |c_n|^2 \quad , \quad (2.45)$$

which means that  $|c_n|^2$  is the probability to have the state  $\varphi_n$  in the state  $\psi$ , and  $c_n = (\varphi_n, \psi)$  is the amplitude of the corresponding probability. This observation was made by Born. We must have

$$(\psi, \psi) = |\psi|^2 = \sum_n |c_n|^2 = 1 \quad (2.46)$$

(since  $\varphi_n$  are orthonormal). Similarly,  $\varphi_n$  is the amplitude of probability of being in state  $n$  (or  $\varphi_n$ ), and  $(\varphi_n, \varphi_n) = |\varphi_n|^2 = 1$  is the probability of being in state  $n$ , which is unity. We can see that the vector  $\psi$  defines the state up to a phase. We note also that the quantum-mechanical operators are linear operators. The expansion given by equation (2.44) means that the eigenvectors  $\varphi_n$  form a complete (or closed) set of vectors, and equation (2.46) is the closure equation.

The matrices (operators) do not commute with one another, in general; we write

$$FG - GF = [F, G] \neq 0 \quad (2.47)$$

for two operators  $F$  and  $G$  that do not commute;  $[F, G]$  is called the commutator of  $F$  and  $G$  (or the commutator of  $F$  with  $G$ ). It is easy to see that if two operators commute, they have common eigenvectors, and if they have common eigenvectors, they commute. This means that they have well-defined values on the same state, they may be simultaneously measured. It follows that the quantum-mechanical state is defined as the common eigenvector of the maximum number

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of commuting operators. This would be the maximum information we may have about the quantum-mechanical motion. The hermitian operators associated to physical quantities are also called observables. A matrix (operator) can be diagonalized, in general; hermitian operators always. The linear transform  $U$  which diagonalizes an operator  $F$  acts like

$$U^{-1}FU = \tilde{F} \quad , \quad (2.48)$$

where  $\tilde{F}$  is diagonal; if  $F$  is hermitian, then  $U^{-1} = U^+$  and  $U^+U = 1$ ; then,  $U$  is called a unitary operator; it may be written as  $U = e^{iS}$ , where  $S$  is hermitian. A unitary transformation preserves the commutation relations.

A convenient notation has been introduced by Dirac, who has written the scalar product as a "bracket"  $(\varphi, \psi) = \langle \varphi | \psi \rangle$ ; then, Dirac called "kets" the vectors  $|\psi\rangle$  and "bras" the vectors  $\langle \varphi |$ . Moreover, Dirac viewed functions of the form  $\varphi_n$ , or  $\varphi(n)$  if  $n$  is continuous, as scalar products  $\langle n | \varphi \rangle$ ; the closure equation (2.46) can be written as

$$\begin{aligned} (\psi, \psi) &= \sum_n |c_n|^2 = \sum_n (c, n)(n, c) = \\ &= \sum_n \langle c | n \rangle \langle n | c \rangle = 1 \quad , \end{aligned} \quad (2.49)$$

whence

$$\sum_n | \langle n | c \rangle |^2 = 1 \quad , \quad (2.50)$$

since  $\langle c | c \rangle = 1$ .

### 2.4.1 Equation of motion

By differentiating equation (2.41) with respect to the time we get

$$\frac{d}{dt}F_{nm} = \frac{i}{\hbar}(E_n - E_m)F_{nm} \quad . \quad (2.51)$$

We may imagine that the states  $n$  are eigenvectors of the hamiltonian  $H$ ,

$$H\varphi_n = E_n\varphi_n \quad (2.52)$$

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(or  $H | n \rangle = E_n | n \rangle$ ); then, removing the scalar products in equation (2.51), we get

$$\frac{dF}{dt} = \frac{i}{\hbar}(HF - FH) = \frac{i}{\hbar}[H, F] ; \quad (2.53)$$

this equation is general; it can also be written as

$$F(t) = e^{\frac{i}{\hbar}Ht} F(0) e^{-\frac{i}{\hbar}Ht} . \quad (2.54)$$

The resemblance of the equation (2.53) with the classical equation of motion

$$\frac{dF}{dt} = \{H, F\} , \quad (2.55)$$

where  $\{\}$  is the Poisson bracket, is striking; to the same extent to which equation (2.55) gives the equations of motion of Newton's Mechanics, equation (2.53) gives the quantum-mechanical equations of motions. The quantum-mechanical equations of motion are given by the commutator with the hamiltonian. These are the canonical equations of motion; for this reason, the unitary transformations which diagonalize hermitian operators (the observables), and preserve the commutation relations, are also called canonical transformations.

The association

$$\frac{i}{\hbar}[H, F] \rightarrow \{H, F\} , \quad [H, F] = -i\hbar\{H, F\} \quad (2.56)$$

was noted by Dirac. It is worth noting that in the limit  $\hbar \rightarrow 0$  the commutator is vanishing: the operators become classical quantities. If the operators have an intrinsic time dependence, not given by the dynamics, then their full equation of motion reads

$$\frac{dF}{dt} = \frac{\partial F}{\partial t} + \frac{i}{\hbar}[H, F] , \quad (2.57)$$

in full analogy with the classical equations of motion.

In scalar products of the form

$$(\varphi, F(t)\psi) = (\varphi, e^{\frac{i}{\hbar}Ht} F(0) e^{-\frac{i}{\hbar}Ht} \psi) \quad (2.58)$$

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we may write

$$\begin{aligned}
 (\varphi, F(t)\psi) &= (\varphi, e^{\frac{i}{\hbar}Ht}F(0)e^{-\frac{i}{\hbar}Ht}\psi) = \\
 &= (e^{-\frac{i}{\hbar}Ht}\varphi, F(0)e^{-\frac{i}{\hbar}Ht}\psi)
 \end{aligned}
 \tag{2.59}$$

and we may imagine that the operators do not depend on the time but, instead, the state vectors do; then we write simply  $F(0) = F$  and

$$\varphi(t) = e^{-\frac{i}{\hbar}Ht}\varphi ; \tag{2.60}$$

which leads to the equation

$$i\hbar \frac{\partial}{\partial t}\varphi(t) = H\varphi(t) ; \tag{2.61}$$

this equation was later called the Schroedinger equation. Time-independent operators and time-dependent state vectors of the form given by equation (2.60) are said to belong to the Schroedinger picture (or Schroedinger representation); while time-dependent operators and time-independent state vectors of the form given by equation (2.58) are said to be in the Heisenberg picture (or Heisenberg representation). If the Heisenberg picture is performed only for the non-interacting part of the hamiltonian, while the interaction is left in the Schroedinger picture, then we say that we have the interaction picture.

We note here that in the above considerations  $H$  is independent of time, as for a closed, conservative motion, and the (constant) energies do exist. The corresponding states are called stationary states. If the hamiltonian depends on the time, then the energy eigenvalues  $E_n(t)$  and the corresponding eigenvectors  $\varphi_n(t)$  depend on the time; although, formally we may define time-dependent frequencies  $\omega(t) = [E_n(t) - E_m(t)]/\hbar$ , the quantization idea of absorbing and emitting such energy differences raises difficulties, since the absorption and emission processes are not instantaneous. However, the Poisson brackets for the classical dynamics are valid, and their quantum-mechanical counterpart with commutators is their expression for finite amounts  $\hbar$  of mechanical action; the classical limit is achieved by these equations of motion in the limit  $\hbar \rightarrow 0$ , so we may maintain the quantum-mechanical equations of motion for time-dependent hamiltonians; the only difference is that expressions like  $Ht$  (in equation

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(2.54), for instance) are replaced by  $\int^t dt' H(t')$  and expressions like  $E_n t$  (in equation (2.41), for instance) are replaced by  $\int^t dt' E_n(t')$ . In addition, the time-dependent Schroedinger equation is satisfied by a linear combination of wavefunctions  $\varphi_n(t)$  with time-dependent coefficients.

Let us consider a particle with mass  $m$  in a potential  $V(\mathbf{r})$ ; the hamiltonian of its motion is

$$H = \frac{1}{2m} p^2 + V(\mathbf{r}) \quad , \quad (2.62)$$

where  $\mathbf{p}$  is momentum. The motion of both the position  $\mathbf{r}$  and the momentum  $\mathbf{p}$  is given by

$$\begin{aligned} \dot{\mathbf{r}} &= \frac{i}{\hbar} [H, \mathbf{r}] = \frac{i}{\hbar} \left[ \frac{1}{2m} p^2, \mathbf{r} \right] = \frac{i}{\hbar} \frac{1}{2m} \{ \mathbf{p}[\mathbf{p}, \mathbf{r}] + [\mathbf{p}, \mathbf{r}]\mathbf{p} \} \quad , \\ \dot{\mathbf{p}} &= \frac{i}{\hbar} [\mathbf{H}, \mathbf{p}] = \frac{i}{\hbar} [V(\mathbf{r}), \mathbf{p}] \quad ; \end{aligned} \quad (2.63)$$

if in the classical limit  $\hbar \rightarrow 0$  we are going to recover the Newton's equations of motion

$$\dot{\mathbf{r}} = \mathbf{p}/m \quad , \quad \dot{\mathbf{p}} = -\frac{\partial V}{\partial \mathbf{r}} \quad (2.64)$$

from the above equations (according to the correspondence principle), we should have

$$[p_x, x] = -i\hbar \quad , \quad [p_x, y] = 0 \quad , \text{etc} \quad ; \quad (2.65)$$

these commutation relations should be read  $[p_i, x_j] = -i\hbar\delta_{ij}$ , where  $i, j$  denote cartesian components. The first Newton's equation follows immediately from the first equation (2.63) and the second Newton's equation follows from the second equation (2.63) by a series expansion. It results that the commutation relations between canonical conjugate variables are the fundamental elements of the quantum-mechanical dynamics.

### 2.4.2 Uncertainty principle

The eigenvalue  $f_n$  in the eigenvalues equation  $F\varphi_n = f_n\varphi_n$  (or  $F | n \rangle = f_n | n \rangle$ ) is the quantity  $F$  we are able to measure (exactly) in