

# Fundamental Principles of Natural Statistical Physics

By

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(Received September 30, 2013)

## Abstract

In this paper, we study the fundamental principles of natural statistical physics. We derive the Schrödinger equations by solving the variational problems for the energy functionals of the physical systems. We give the many solutions of the natural statistical physics. At last we give several unsolved problems of the natural statistical physics. As for the precise, we refer to the references.

2010 Mathematics Subject Classification. Primary 81P99.

## Introduction

In this paper, we established the fundamental principles of natural statistical physics.

The theory of natural statistical physics is different from the quantum mechanics.

In this theory, we study the phenomena of electrons, atoms and molecules as the statistical phenomena of the family of these micro-particles. These phenomena are governed by the laws of natural statistical physics. We give the

three cases of the laws of natural statistical physics. We need the marginal distribution law in order to calculate the expectation value of angular momentum. Thus we give one case of the marginal distribution law.

In order to study the state of a physical system, we need the  $L^2$ -density or the  $L^2_{loc}$ -density which is the solution of the Schrödinger equation.

We derive the Schrödinger equation of the physical system as the solution of variational problem on the basis of the variational principles. We give the three cases of the derivations of the Schrödinger equations. We show the solutions of the problems of natural statistical physics. We have already those solutions in many cases of the natural statistical phenomena. At last we give several unsolved problems of the natural statistical phenomena. As the reference, we give the table of correspondence of new and old terminologies in this theory.

From now on, it is the problem to analyze the concrete natural statistical phenomena by using this new theory.

At last, I express my heartfelt thanks to my wife Mutuko for her helping me the work of typesetting of the manuscript.

## 1 Fundamental problems of natural statistical physics

In the natural statistical physics, we understand the physical phenomena on the bases of statistical quantities such as the expectation values or mean values of physical quantities of a certain physical system. Then, the physical quantities of the physical system are the functions of the position variables and the momentum variables. Therefore, in order to understand the natural statistical phenomena of this physical system, we have to know the natural probability distribution states of the position variables and the momentum variables of this physical system.

By virtue of the laws of the natural statistical physics, if we determine the  $L^2$ -density  $\psi$  determining the natural probability distribution law of the position variables of this physical system, the natural probability distribution law of the momentum variables of this physical system is determined by its Fourier transform  $\hat{\psi}$ .

By virtue of the laws of the natural statistical physics, this  $L^2$ -density  $\psi$  is the solution of Schrödinger equation of this physical system. Therefore, in order to study the natural statistical phenomena of this physical system, the fundamental problem is to solve the Schrödinger equation as the fundamental equation. Thus the natural statistical phenomena can be understood on the bases of the laws of the natural statistical physics.

In the following sections, we postulate the laws of the natural statistical physics.

## 2 Laws of natural statistical physics

In this section, we postulate the laws of natural statistical physics. Here we consider the case where the Schrödinger operator has only the discrete spectrum.

When we study the natural statistical phenomena using the natural statistical physics, we postulate the following three concepts :

- (1) The physical system.
- (2) The state of the physical system.
- (3) The motion of the physical system.

We call these postulations to be the laws of natural statistical physics. These laws are the natural laws of natural statistical phenomena.

The laws of natural statistical physics are described in the following way. As for these facts, we refer to Ito [1], [5], [6], [8], [9], [13]~[20], [22], [24], Ito-Kayama [1], [2], Ito-Kayama-Kamosita [1], and Ito-Uddin [1], [2].

The laws of natural statistical physics are formulated in Ito [5] at first time. This gives the mathematical expression to the statement of natural statistical physics in Ito [8]. These laws were completely expressed in the form in Ito [15].

**Law I (physical system)** We postulate that the physical system  $\Omega$  is a probability space  $\Omega = \Omega(\mathcal{B}, P) = (\Omega, \mathcal{B}, P)$ . Here  $\Omega$  is the set of the systems  $\rho$  of micro-particles,  $\mathcal{B}$  is a  $\sigma$ -algebra composed of the subsets of  $\Omega$ , and  $P$  is a completely additive probability measure.

**Law II (state of the physical system)** We postulate that the state of the physical system  $\Omega$  is defined to be the natural probability distributions of the position variable  $\mathbf{r}(\rho)$  and the momentum variable  $\mathbf{p}(\rho)$  of the system of the micro-particles  $\rho \in \Omega$ . Here  $\mathbf{r}(\rho)$  moves in  $n$ -dimensional space  $\mathbf{R}^n$  and  $\mathbf{p}(\rho)$  moves in its dual space  $\mathbf{R}_n$ . Here we put  $n = Md$ ,  $d$  denoting the dimension of the physical space and  $M$  denoting the number of micro-particles which compose an elementary event  $\rho$ . Then, because the space  $\mathbf{R}^n$  is self-dual, we identify  $\mathbf{R}_n$  with  $\mathbf{R}^n$ .

(i) We postulate that the natural probability distribution of the position variable  $\mathbf{r} = \mathbf{r}(\rho)$  is determined by an  $L^2$ -density  $\psi(\mathbf{r})$  defined on  $\mathbf{R}^n$ .

(ii) We postulate that the natural probability distribution of the momentum variable  $\mathbf{p} = \mathbf{p}(\rho)$  is determined by its Fourier transform  $\hat{\psi}(\mathbf{r})$ . Here, we put

$$\hat{\psi}(\mathbf{p}) = \frac{1}{(\sqrt{2\pi\hbar})^n} \int \psi(\mathbf{r}) e^{-i(\mathbf{p}\cdot\mathbf{r})/\hbar} d\mathbf{r},$$

$$\psi(\mathbf{r}) = \frac{1}{(\sqrt{2\pi\hbar})^n} \int \hat{\psi}(\mathbf{p}) e^{i(\mathbf{p}\cdot\mathbf{r})/\hbar} d\mathbf{p},$$

$$\mathbf{r} = {}^t(x_1, x_2, \dots, x_n), \quad \mathbf{p} = {}^t(p_1, p_2, \dots, p_n),$$

$$\mathbf{p} \cdot \mathbf{r} = p_1 x_1 + p_2 x_2 + \dots + p_n x_n.$$

Here we put  $\hbar = \frac{h}{2\pi}$ , where  $h$  denotes Planck's constant. Here the integral denotes the Lebesgue integral on the whole space  $\mathbf{R}^n$  when the integration domain is not expressed clearly. In the sequel, the similar notation is used.

(iii) We postulate that, for a Lebesgue measurable set  $A$  in  $\mathbf{R}^n$ ,

$$\mu(A) = \int_A |\psi(\mathbf{r})|^2 d\mathbf{r}$$

denotes the probability of the event “ $\mathbf{r}(\rho)$  belongs to  $A$ ”. Then we have

$$P(\{\rho \in \Omega; \mathbf{r}(\rho) \in A\}) = \mu(A).$$

Thereby we have the probability space  $(\mathbf{R}^n, \mathcal{M}_n, \mu)$ . Here  $\mathcal{M}_n$  denotes the family of all Lebesgue measurable sets in  $\mathbf{R}^n$ .

(iv) We postulate that, for a Lebesgue measurable set  $B$  in  $\mathbf{R}^n$ ,

$$\nu(B) = \int_B |\hat{\psi}(\mathbf{p})|^2 d\mathbf{p}$$

denotes the probability of the event “ $\mathbf{p}(\rho)$  belongs to  $B$ ”. Then we have

$$P(\{\rho \in \Omega; \mathbf{p}(\rho) \in B\}) = \nu(B).$$

Thereby we have the probability space  $(\mathbf{R}^n, \mathcal{N}_n, \nu)$ . Here  $\mathcal{N}_n$  denotes the family of all Lebesgue measurable sets in  $\mathbf{R}^n$ .

The reason why we define the Fourier transformation in such a form in Law (II), (ii) is to meet with the necessity that the Schrödinger equation of the physical system should be derived by using the variational principle in section 6. The constants are chosen in order that the theoretical results coincide with some observed data of the natural statistical phenomena.

**Law III (motion of the physical system)** We postulate that the  $L^2$ -density  $\psi(\mathbf{r}, t)$  determining the natural probability distribution law of the position variable  $\mathbf{r}$  at time  $t$  is determined by the time evolving Schrödinger equation. We call this time evolution the motion of the physical system. The law of motion of the physical system is described by the Schrödinger equation. We call this Schrödinger equation the equation of motion of the physical system.

The Schrödinger equation is described in the following form :

$$i\hbar \frac{\partial \psi}{\partial t} = H\psi.$$

We call the operator  $H$  a Schrödinger operator.  $H$  is a self-adjoint operator on a certain Hilbert space. The concrete form of this operator is determined for every concrete physical system.

### 3 Laws of generalized natural probability distribution

In this section, we postulate the laws of generalized natural probability distribution. Here we consider the case where the Schrödinger operator has the continuous spectrum.

The laws of generalized natural probability distributions are formulated in Ito [26] at first time.

**Law I' ((generalized) proper physical subsystem)** We postulate that the proper physical subsystem or the generalized proper physical subsystem  $\Omega'$  is a physical subsystem which is a probability subspace of the total physical system  $(\Omega, \mathcal{B}, P)$ . Here  $\Omega$  is the set of the system  $\rho$  of micro-particles,  $\mathcal{B}$  is a  $\sigma$ -algebra composed of the subsets of  $\Omega$ , and  $P$  is a completely additive probability measure.

Then this satisfies the law II' of the state of generalized proper physical subsystem and the law III' of the motion of generalized proper physical subsystem in the following.

**Law II' (state of the (generalized) proper physical subsystem) (1)**

When the Schrödinger operator has only the discrete spectrum, we postulate that the state of the proper physical subsystem  $\Omega'$  is determined by using the eigenfunction  $\psi$  of the Schrödinger operator in the same way as Law II in section 2.

(2) When the Schrödinger operator has the continuous spectrum, we postulate that the state of the generalized proper physical subsystem  $\Omega'$  is determined by using the generalized eigenfunction  $\psi$  of the Schrödinger operator in the following :

(i)' We postulate that the generalized natural probability distribution of the position variable  $\mathbf{r} = \mathbf{r}(\rho)$  is determined by an  $L^2_{\text{loc}}$ -density  $\psi(\mathbf{r})$  defined on  $\mathbf{R}^n$ .

(ii)' We postulate that the generalized natural probability distribution of the momentum variable  $\mathbf{p} = \mathbf{p}(\rho)$  is determined by its Fourier transform  $\hat{\psi}(\mathbf{p})$ . Here,  $\hat{\psi}$  is the Fourier transform of  $\psi$  defined by the relation :

$$\hat{\psi}(\mathbf{p}) = \lim_{R \rightarrow \infty} \hat{\psi}_S(\mathbf{p}),$$

where the limit is taken in the sense of generalized functions.

In the above formula, we use the local Fourier transform  $\hat{\psi}_S$  defined in the following way :

$$\hat{\psi}_S(\mathbf{p}) = \frac{1}{(\sqrt{2\pi\hbar})^n} \int \psi_S(\mathbf{r}) e^{-i(\mathbf{p}\cdot\mathbf{r})/\hbar} d\mathbf{r},$$

$$\psi_S(\mathbf{r}) = \frac{1}{(\sqrt{2\pi\hbar})^n} \int \hat{\psi}_S(\mathbf{p}) e^{i(\mathbf{p}\cdot\mathbf{r})/\hbar} d\mathbf{p},$$

$$\mathbf{r} = {}^t(x_1, x_2, \dots, x_n), \quad \mathbf{p} = {}^t(p_1, p_2, \dots, p_n),$$

$$\mathbf{p} \cdot \mathbf{r} = p_1 x_1 + p_2 x_2 + \dots + p_n x_n.$$

Here, for arbitrary compact set  $S$  in  $\mathbf{R}^n$ ,  $\psi_S$  denotes the section of  $\psi$  on the closed sphere  $S = \{\|\mathbf{r}\| \leq R\}$  of the radius  $R > 0$ . Namely,  $\psi_S(\mathbf{r})$  is defined by the relation  $\psi_S(\mathbf{r}) = \psi(\mathbf{r})\chi_S(\mathbf{r})$ . Here  $\chi_S(\mathbf{r})$  denotes the characteristic function of the closed sphere  $S = \{\|\mathbf{r}\| \leq R\}$  of the radius  $R > 0$ . Further we put  $\hbar = \frac{h}{2\pi}$ , where  $h$  denotes Planck's constant.

(iii)' We postulate that, for a Lebesgue measurable set  $A$  in  $\mathbf{R}^n$ ,

$$\mu_S(A) = \frac{\int_{A \cap S} |\psi_S(\mathbf{r})|^2 d\mathbf{r}}{\int_S |\psi_S(\mathbf{r})|^2 d\mathbf{r}}$$

denotes the probability of the event " $\mathbf{r}(\rho)$  of a system  $\rho$  of micro-particles moving in the region  $S$  belongs to  $A \cap S$ ". Then we have

$$P(\{\rho \in \Omega; \mathbf{r}(\rho) \in A \cap S\}) = \mu_S(A).$$

Thereby we have the relative probability space  $(\mathbf{R}^n, \mathcal{M}_n \cap S, \mu_S)$  corresponding to  $\psi_S$ . Here  $\mathcal{M}_n$  denotes the family of all Lebesgue measurable sets in  $\mathbf{R}^n$ .

(iv)' We postulate, for a Lebesgue measurable set  $B$  in  $\mathbf{R}^n$ ,

$$P(\{\rho \in \Omega; \mathbf{r}(\rho) \in S, \mathbf{p}(\rho) \in B\}) = \nu_S(B)$$

denotes the probability of the event " $\mathbf{p}(\rho)$  of a system  $\rho$  of micro-particles moving in the region  $S$  belongs to  $B$ ". Then we have

$$\nu_S(B) = \frac{\int_B |\hat{\psi}_S(\mathbf{p})|^2 d\mathbf{p}}{\int |\hat{\psi}_S(\mathbf{p})|^2 d\mathbf{p}}.$$

Thereby we have the relative probability space  $(\mathbf{R}^n, \mathcal{N}_n, \nu_S)$  corresponding to  $\psi_S$ . Here  $\mathcal{N}_n$  denotes the family of all Lebesgue measurable sets in  $\mathbf{R}^n$ .

The reason why we define the Fourier transformation in such a form in Law (II)', (ii)' is to meet with the necessity that the Schrödinger equation of the physical system should be derived by using the variational principle in section 7. The constants are chosen in order that the theoretical results coincide with some observed data of the natural statistical phenomena.

**Law III' (motion of the physical subsystem)** We postulate that the  $L^2$ -density  $\psi(\mathbf{r}, t)$  determining the natural probability distribution law of the position variable  $\mathbf{r}$  at time  $t$  is determined by the time evolving Schrödinger equation. We call this time evolution the motion of the physical system. The law of motion of the physical system is described by the Schrödinger equation. We call this Schrödinger equation the equation of motion of the physical system.

The Schrödinger equation is described in the following form :

$$i\hbar \frac{\partial \psi}{\partial t} = H\psi.$$

We call the operator  $H$  a Schrödinger operator.  $H$  is a self-adjoint operator on a certain Hilbert space. The concrete form of this operator is determined for every concrete physical system.

## 4 Laws of natural statistical physics concerning the periodic motion

In this section, we postulate the laws of natural statistical physics concerning the periodic motion.

**Law I (physical system)** We postulate that the physical system  $\Omega$  is a probability space  $\Omega = \Omega(\mathcal{B}, P) = (\Omega, \mathcal{B}, P)$ . Here  $\Omega$  is the set of the system  $\rho$  of micro-particles,  $\mathcal{B}$  is a  $\sigma$ -algebra composed of the subsets of  $\Omega$ , and  $P$  is a completely additive probability measure.

Each system of micro-particles  $\rho$  moves periodically on the interval  $D = [-a, a]^n$ . Its fundamental period is  $2a$  in each direction of orthogonal axes.

**Law II (state of the physical system)** We postulate that the state of the physical system  $\Omega = \Omega(\mathcal{B}, P) = (\Omega, \mathcal{B}, P)$  is defined to be the natural probability distributions of the position variable  $\mathbf{r}(\rho)$  and the momentum variable  $\mathbf{p}(\rho)$  of the system of micro-particles  $\rho \in \Omega$ . Here  $\mathbf{r}(\rho)$  moves periodically on the interval  $D = [-a, a]^n$  in  $n$ -dimensional space  $\mathbf{R}^n$  and  $\mathbf{p}(\rho)$  moves in its dual space  $\mathbf{P}_n$  which is the countable set of  $n$ -column vectors whose components are integers. Here we put  $n = Md$ ,  $d$  denoting the dimension of the physical space and  $M$  denoting the number of micro-particles which compose an elementary event  $\rho$ .

(i) We postulate that the natural probability distribution of the position variable  $\mathbf{r} = \mathbf{r}(\rho)$  is determined by an  $L^2$ -density  $\psi(\mathbf{r})$  defined on  $D$ .

Here  $\psi(\mathbf{r})$  satisfies the periodic boundary conditions

$$\psi(\mathbf{r})|_{x_j=-a} = \psi(\mathbf{r})|_{x_j=a}, \quad (\mathbf{r} \in D, j = 1, 2, \dots, n)$$

and the normalization condition

$$\int_D |\psi(\mathbf{r})|^2 d\mathbf{r} = 1.$$

(ii) We postulate that the natural probability distribution of the momentum variable  $\mathbf{p} = \mathbf{p}(\rho)$  is determined by its Fourier coefficients  $\hat{\psi}(\mathbf{p})$ . Here we put

$$\hat{\psi}(\mathbf{p}) = \frac{1}{(\sqrt{2a\hbar})^n} \int_D \psi(\mathbf{r}) e^{-i(\mathbf{p}\cdot\mathbf{r})/\hbar} d\mathbf{r},$$

$$\psi(\mathbf{r}) = \frac{1}{(\sqrt{2a\hbar})^n} \sum_{\mathbf{p} \in \mathbf{P}_n} \hat{\psi}(\mathbf{p}) e^{i(\mathbf{p}\cdot\mathbf{r})/\hbar},$$

$$\int_D |\psi(\mathbf{r})|^2 d\mathbf{r} = \sum_{\mathbf{p} \in \mathbf{P}_n} |\hat{\psi}(\mathbf{p})|^2 = 1.$$

$$\mathbf{r} = {}^t(x_1, x_2, \dots, x_n), \quad \mathbf{p} = {}^t(p_1, p_2, \dots, p_n),$$

$$\mathbf{p} \cdot \mathbf{r} = p_1 x_1 + p_2 x_2 + \dots + p_n x_n.$$

Here we put  $\hbar = \frac{h}{2\pi}$ , where  $h$  denotes Planck's constant.

(iii) We postulate that, for a Lebesgue measurable set  $A$  in  $D = [-a, a]^n$ ,

$$\mu(A) = \int_A |\psi(\mathbf{r})|^2 d\mathbf{r}$$



denotes the probability of the event “ $\mathbf{r}(\rho)$  belongs to  $A$ ”. Then we have

$$P(\{\rho \in \Omega; \mathbf{r}(\rho) \in A\}) = \mu(A).$$

Thereby we have the probability space  $(D, \mathcal{M}_n, \mu)$ . Here  $\mathcal{M}_n$  denotes the family of all Lebesgue measurable sets in  $D$ .

(iv) We postulate that, for any subset  $B$  in  $\mathbf{P}_n$ ,

$$\nu(B) = \sum_{\mathbf{p} \in B} |\hat{\psi}(\mathbf{p})|^2$$

denotes the probability of the event “ $\mathbf{p}(\rho)$  belongs to  $B$ ”. Then we have

$$P(\{\rho \in \Omega; \mathbf{p}(\rho) \in B\}) = \nu(B).$$

Thereby we have the probability space  $(\mathbf{P}_n, \mathcal{N}_n, \nu)$ . Here  $\mathcal{N}_n$  denotes the family of all subsets in  $\mathbf{P}_n$ .

The reason why we define the Fourier coefficient in such a form in Law (II), (ii) is to meet with the necessity that the Schrödinger equation of the physical system should be derived by using the variational principle in section 8. The constants are chosen in order that the theoretical results coincide with some observed data of the natural statistical phenomena.

**Law III (motion of the physical system)** We postulate that the  $L^2$ -density  $\psi(\mathbf{r}, t)$  determining the natural probability distribution law of the position variable  $\mathbf{r}$  at time  $t$  is determined by the time evolving Schrödinger equation. We call this time evolution the motion of the physical system. The law of motion of the physical system is described by the Schrödinger equation. We call this Schrödinger equation the equation of motion of the physical system.

The Schrödinger equation is described in the following form :

$$i\hbar \frac{\partial \psi}{\partial t} = H\psi.$$

We call the operator  $H$  a Schrödinger operator.  $H$  is a self-adjoint operator on a certain Hilbert space. The concrete form of this operator is determined for every concrete physical system.

Here  $\psi(\mathbf{r}, t)$  satisfies the following initial and boundary conditions :

$$\psi(\mathbf{r}, 0) = \psi(\mathbf{r}), \quad (\mathbf{r} \in D), \quad (\text{Initial condition})$$

$$\begin{aligned} \psi(\mathbf{r})|_{x_j=-a} &= \psi(\mathbf{r})|_{x_j=a}, \quad \psi(\mathbf{r}, t)|_{x_j=-a} = \psi(\mathbf{r}, t)|_{x_j=a}, \\ (\mathbf{r} \in D, \quad 0 < t < \infty), \quad (j = 1, 2, \dots, n), \end{aligned}$$

(periodic boundary conditions).

Here,  $\psi(\mathbf{r})$  is a given  $L^2$ -density.

When  $H$  contains a potential  $V(\mathbf{r})$ , we assume that it satisfies the periodic boundary conditions

$$V(\mathbf{r})|_{x_j=-a} = V(\mathbf{r})|_{x_j=a}, \quad (\mathbf{r} \in D, j = 1, 2, \dots, n).$$

## 5 Marginal distribution law

In this section we study the concept of marginal distribution law.

When we study the expectation values of angular momenta of the system of inner electrons of hydrogen atoms, we need the concept of marginal distribution law.

At first, we give a mathematical model for the system of hydrogen atoms. We consider the system of hydrogen atoms as the family of hydrogen atoms, each electron of which is moving in the Coulomb potential

$$V(r) = -\frac{e^2}{r}, \quad (r = \|\mathbf{r}\|)$$

with its center at the nucleus of the hydrogen atom.

Each electron is moving according to Newtonian equation of motion by virtue of the causality laws.

As a mathematical model, this physical system is the system of inner electrons of hydrogen atoms which are moving in the Coulomb potential with its center at the origin.

We denote this system of inner electrons of hydrogen atoms by  $\Omega = \Omega(\mathcal{B}, P)$ . In this paper, we call this physical system to be the system of hydrogen atoms.

Each electron  $\rho$  has its position variable  $\mathbf{r} = \mathbf{r}(\rho)$  and its momentum variable  $\mathbf{p} = \mathbf{p}(\rho)$ . Here we postulate that the variables  $\mathbf{r} = \mathbf{r}(\rho)$  and  $\mathbf{p} = \mathbf{p}(\rho)$  are the vector valued random variables defined on  $\Omega$ .

In this case, each electron  $\rho$  has the total energy

$$\mathcal{E}(\rho) = \frac{1}{2m_e} \mathbf{p}(\rho)^2 - \frac{e^2}{r},$$

where  $m_e$  and  $e$  denote the mass and the electric charge of the electron respectively.

We calculate the expectation value of the angular momentum of the system of inner electrons of hydrogen atoms

$$\mathbf{L} = \mathbf{r} \times \mathbf{p} = {}^t(L_x, L_y, L_z).$$

By virtue of the laws of natural statistical physics, the probability distribution law of the variable  $\mathbf{r} = \mathbf{r}(\rho)$  is determined by the  $L^2$ -density  $\psi$  which is a solution of Schrödinger equation of the system of hydrogen atoms

$$i\hbar \frac{\partial \psi(\mathbf{r}, t)}{\partial t} = \left( -\frac{\hbar^2}{2m_e} \Delta - \frac{e^2}{r} \right) \psi(\mathbf{r}, t).$$

Then the probability distribution law of the variable  $\mathbf{p} = \mathbf{p}(\rho)$  is determined by its Fourier transform  $\hat{\psi}$ .

Here we define the Fourier transformation of  $\psi$  as follows:

$$\hat{\psi}(\mathbf{p}) = \frac{1}{(\sqrt{2\pi\hbar})^3} \int \psi(\mathbf{r}) e^{-i(\mathbf{p}\cdot\mathbf{r})/\hbar} d\mathbf{r},$$

where we put

$$\mathbf{r} = {}^t(x, y, z), \quad \mathbf{p} = {}^t(p_x, p_y, p_z), \quad \mathbf{p} \cdot \mathbf{r} = p_x x + p_y y + p_z z.$$

Here we give the fundamental relations in the natural probability distribution laws in the following:

$$P(\{\rho \in \Omega; \mathbf{r}(\rho) \in A\}) = \int_A |\psi(\mathbf{r})|^2 d\mathbf{r},$$

and

$$P(\{\rho \in \Omega; \mathbf{p}(\rho) \in B\}) = \int_B |\hat{\psi}(\mathbf{p})|^2 d\mathbf{p}.$$

Here  $A$  and  $B$  are Lebesgue measurable sets in  $\mathbf{R}^3$ .

Further the natural probability distribution law of the variable  $(x(\rho), p_y(\rho))$  is determined by the partial Fourier transform  $\hat{\psi}(x, p_y, z)$  as the marginal distribution of the simultaneous distribution of the variables  $(x(\rho), p_y(\rho), z(\rho))$ .

Here the partial transformation of  $\psi$  is defined in the following relation:

$$\hat{\psi}(x, p_y, z) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \psi(x, y, z) e^{-ip_y y/\hbar} dy.$$

The other marginal distributions are defined similarly.

Thereby, by using the natural probability distribution law of the variable  $(x(\rho), p_y(\rho))$  as the marginal distribution, the expectation value of the  $z$ -component  $L_z$  of the angular momentum is calculated by the following formula

$$E[L_z] = \int_{\Omega} L_z(\rho) dP(\rho) = \frac{\hbar}{i} \int \overline{\psi(\mathbf{r})} \left( x \frac{\partial}{\partial y} - y \frac{\partial}{\partial x} \right) \psi(\mathbf{r}) d\mathbf{r}.$$

In the right hand side of the above equality, the operator expression is formal and used only for the benefit of the mathematical calculation. Further, we remark that this operator expression has no physical meaning.

For  $L_x, L_y, L^2 = L_x^2 + L_y^2 + L_z^2$ , we calculate their expectation values in the same way.

We remark that the partial derivatives of the  $L^2$ -functions  $\psi$  are calculated in the sense of  $L^2$ -convergence. We call these the partial  $L^2$ -derivatives of  $\psi$ .

## 6 Solutions of variational problems

In this section, we study the solutions of variational problems in order to derive the Schrödinger equations. For the precise, we refer to Ito [12], section 3.2.

Hamiltonian  $H$  appeared in the Schrödinger equation which describes the natural statistical phenomena of the physical system considered here has, generally, the form

$$H = - \sum_{i=1}^n \frac{\hbar^2}{2m_i} \frac{\partial^2}{\partial x_i^2} + V.$$

Here,  $m_i$ , ( $1 \leq i \leq n$ ) denote the masses of the micro-particles. The values of  $m_i$  corresponding to one micro-particle are the same.  $V$  denotes the potential.

We call this operator  $H$  the **Hamiltonian operator**. In other word, we also call this the **Schrödinger operator**.

In this section, especially, we study the solution of the variational problem when this Schrödinger operator  $H$  has only the discrete spectrum.

Let  $\mathbf{R}^n$  be the  $n$ -dimensional space. Here we assume  $n \geq 1$ .

Now we consider one physical system  $\Omega = \Omega(\mathcal{B}, P)$ . Mathematically, we consider that this is a probability space. Its elementary event  $\rho$  is one system of micro-particles. Its position variable is  $\mathbf{r} = \mathbf{r}(\rho) = {}^t(x_1(\rho), x_2(\rho), \dots, x_n(\rho))$  and its momentum variable is  $\mathbf{p} = \mathbf{p}(\rho) = {}^t(p_1(\rho), p_2(\rho), \dots, p_n(\rho))$ .

We consider that the variable  $\mathbf{r}$  moves in  $\mathbf{R}^n$  and the variable  $\mathbf{p}$  moves in its dual space  $\mathbf{R}^n$ . Here, because the space  $\mathbf{R}^n$  is self-dual, we identifies the dual space  $\mathbf{R}_n$  with the space  $\mathbf{R}^n$ .

Then, by virtue of the law II in Ito [12], section 2.2, the  $L^2$ -density  $\psi(\mathbf{r})$  determines the natural probability distribution law of the position variable  $\mathbf{r}$  and its Fourier transform  $\hat{\psi}(\mathbf{p})$  determines the natural probability distribution law of the momentum variable  $\mathbf{p}$ .

We assume that the potential  $V(\mathbf{r})$  is a real-valued measurable function on  $\mathbf{R}^n$ .

Then we define the **energy functional**  $J[\psi]$  of  $L^2$ -density  $\psi(\mathbf{r})$  by the relation

$$J[\psi] = \int \left( \sum_{i=1}^n \frac{\hbar^2}{2m_i} \left| \frac{\partial \psi(\mathbf{r})}{\partial x_i} \right|^2 + V(\mathbf{r}) |\psi(\mathbf{r})|^2 \right) d\mathbf{r}.$$

Here the integral denotes the Lebesgue integral on the whole space  $\mathbf{R}^n$  when the integration domain is not expressed clearly.

In the sequel, we consider the integral similarly.

In this section, the partial derivatives of  $L^2$ -functions are defined in the sense of  $L^2$ -convergence. As for the precise, we refer to Ito [29], [34].

The domain of  $J[\psi]$  is the Hilbert space of all  $L^2$ -functions  $\psi$  given by the relation

$$\mathbb{D} = \left\{ \psi \in L^2; \int |\nabla\psi(\mathbf{r})|^2 d\mathbf{r} < \infty, \right. \\ \left. \int |V(\mathbf{r})||\psi(\mathbf{r})|^2 d\mathbf{r} < \infty \right\}$$

Here  $\nabla = \nabla_{\mathbf{r}}$  denotes the gradient operator.

$\mathbb{D}$  is the metric space with the metric

$$r(\psi, \psi') = \|\psi' - \psi\|$$

defined by the following norm

$$\|\psi\|^2 = \int (|\psi(\mathbf{r})|^2 + |\nabla\psi(\mathbf{r})|^2 + |V(\mathbf{r})||\psi(\mathbf{r})|^2) d\mathbf{r}.$$

Here we use the notation

$$|\nabla\psi(\mathbf{r})|^2 = \sum_{i=1}^n \left| \frac{\partial\psi(\mathbf{r})}{\partial x_i} \right|^2.$$

Now we assume that  $\mathcal{D} = \mathcal{D}(\mathbf{R}^n)$  is the space of all  $C^\infty$ -functions with compact support in  $\mathbf{R}^n$  and  $\mathcal{D}$  is dense in  $\mathbb{D}$ .

$J[\psi]$  is the continuous functional on  $\mathbb{D}$ .

Then we study the variational problem in the following.

**Problem I (variational problem)** We use the notation in the above. Then determine the stationary function  $\psi$  of the energy functional  $J[\psi]$  defined on  $\mathbb{D}$ . Here we assume that  $\psi \in \mathbb{D}$  satisfies the condition

$$\int |\psi(\mathbf{r})|^2 d\mathbf{r} = 1.$$

Now, if we put

$$K[\psi] = \int |\psi(\mathbf{r})|^2 d\mathbf{r},$$

the variational problem I in the above is the stationary value problem of  $J[\psi]$  under the condition

$$K[\psi] = 1.$$

Therefore we determine the stationary function using the Lagrange's method of indeterminate coefficients.

$\mathcal{E}$  being a Lagrange's indeterminate coefficient, we put

$$I[\psi] = J[\psi] - \mathcal{E}(K[\psi] - 1).$$

Then the conditional stationary value problem in the above is equivalent to the stationary value problem of  $I[\psi]$ .

Now, assume that we have a solution  $\psi$  of the conditional stationary problem in the above. Then this  $\psi$  is the stationary function of  $I[\psi]$ .

Then,  $\varepsilon$  being a sufficiently small real parameter, we have

$$\frac{d}{d\varepsilon}(I[\psi + \varepsilon\varphi])|_{\varepsilon=0} = 0, \quad (1)$$

$$\frac{d}{d\varepsilon}(I[\psi + i\varepsilon\varphi])|_{\varepsilon=0} = 0 \quad (2)$$

for any  $\varphi \in \mathbb{D}$ .

Then, by the formulas (1), (2), we have the equality

$$\sum_{i=1}^n \frac{\hbar^2}{2m_i} \left( \frac{\partial\varphi}{\partial x_i}, \frac{\partial\psi}{\partial x_i} \right) + (\varphi, V\psi) - (\varphi, \mathcal{E}\psi) = 0.$$

Here  $(\cdot, \cdot)$  denotes the inner product in  $L^2$ .

Using Plancherel's equality twice in the first term in this formula, we have the equality

$$\left( \varphi, - \sum_{i=1}^n \frac{\hbar^2}{2m_i} \frac{\partial^2\psi}{\partial x_i^2} + V\psi - \mathcal{E}\psi \right) = 0.$$

Because this formula holds for any  $\varphi \in \mathcal{D}$ , we have

$$- \sum_{i=1}^n \frac{\hbar^2}{2m_i} \frac{\partial^2\psi}{\partial x_i^2} + V\psi = \mathcal{E}\psi. \quad (3)$$

When we have a solution  $\psi \in \mathbb{D}$  which is not identically zero for the eigenvalue problem (3), we say that  $\mathcal{E}$  and  $\psi$  are the **eigenvalue** and the **eigenfunction** of the Schrödinger operator

$$H = - \sum_{i=1}^n \frac{\hbar^2}{2m_i} \frac{\partial^2}{\partial x_i^2} + V$$

respectively. Especially,  $\psi$  is the eigenfunction belonging to the eigenvalue  $\mathcal{E}$ .

This eigenvalue problem for the Schrödinger operator  $H$  is the fundamental problem of the natural statistical physics as the generalization of the eigenvalue problem for the Sturm-Liouville operator to the case of several variables.

This is the **Euler differential equation** for the conditional variational problem. We call this the **Schrödinger equation**.

This Schrödinger equation is the necessary condition in order to the existence of the solution of the variational problem I in the above. For the concrete physical system, we can prove the completeness of the system of eigenfunctions of this eigenvalue problem.

Then, because we can determine the  $L^2$ -density for the total physical system completely by the eigenfunction expansion, we can solve this Schrödinger equation completely.

In this sense, by solving the Schrödinger equation obtained here, we can obtain the information on the natural probability distribution state of the physical system.

## 7 Solutions of local variational problems

In this section, we study the solutions of local variational problems in order to derive the Schrödinger equations. For the precise, we refer to Ito [12], section 3.2.

In this section, especially, we study the solution of the local variational problem when this Schrödinger operator  $H$  has a continuous spectrum.

Let  $\mathbf{R}^n$  be the  $n$ -dimensional space. Here we assume  $n \geq 1$ .

Now we consider one physical system  $\Omega = \Omega(\mathcal{B}, P)$ . Mathematically, we consider that this is a probability space. Its elementary event  $\rho$  is one system of micro-particles. Its position variable is  $\mathbf{r} = \mathbf{r}(\rho) = {}^t(x_1(\rho), x_2(\rho), \dots, x_n(\rho))$  and its momentum variable is  $\mathbf{p} = \mathbf{p}(\rho) = {}^t(p_1(\rho), p_2(\rho), \dots, p_n(\rho))$ .

We consider that the variable  $\mathbf{r}$  moves in  $\mathbf{R}^n$  and the variable  $\mathbf{p}$  moves in its dual space  $\mathbf{R}^n$ . Here, because the space  $\mathbf{R}^n$  is self-dual, we identifies the dual space  $\mathbf{R}_n$  with the space  $\mathbf{R}^n$ .

Then, by virtue of the law I', the law II' and the law III' in Ito [12], section 2.5, the  $L^2_{\text{loc}}$ -density  $\psi(\mathbf{r})$  determines the generalized natural probability distribution law of the position variable  $\mathbf{r}$  and its Fourier transform  $\hat{\psi}(\mathbf{p})$  determines the generalized natural probability distribution law of the momentum variable  $\mathbf{p}$ .

We assume that the potential  $V(\mathbf{r})$  is a real-valued measurable function on  $\mathbf{R}^n$ .

We assume that  $S$  is a certain compact set in  $\mathbf{R}^n$  and  $S$  is not a null-set.

Then, for a certain  $L^2_{\text{loc}}$ -density  $\psi(\mathbf{r})$  defined on  $\mathbf{R}^n$ , we put

$$\psi_S(\mathbf{r}) = \psi(\mathbf{r})\chi_S(\mathbf{r}).$$

Here  $\chi_S(\mathbf{r})$  is the characteristic function of  $S$ .

Then we define the **local energy functional**  $J_S[\psi_S]$  by the relation

$$J_S[\psi_S] = \frac{\int_S \left( \sum_{i=1}^n \frac{\hbar^2}{2m_i} \left| \frac{\partial \psi_S(\mathbf{r})}{\partial x_i} \right|^2 + V(\mathbf{r}) |\psi_S(\mathbf{r})|^2 \right) d\mathbf{r}}{\int_S |\psi_S(\mathbf{r})|^2 d\mathbf{r}}.$$

In this section, the partial derivatives of  $L_{\text{loc}}^2$ -functions are defined in the sense of  $L_{\text{loc}}^2$ -convergence.

The domain  $\mathbb{D}$  of  $J_S[\psi_S]$  is the Hilbert space

$$\mathbb{D} = \left\{ \psi_S \in L^2(S); \int_S |\nabla \psi_S(\mathbf{r})|^2 d\mathbf{r} < \infty, \right. \\ \left. \int_S |V(\mathbf{r})| |\psi_S(\mathbf{r})|^2 d\mathbf{r} < \infty \right\}.$$

The norm  $\|\psi_S\|$  of  $\mathbb{D}$  is defined by the following relation

$$\|\psi_S\|^2 = \int_S (|\psi_S(\mathbf{r})|^2 + |\nabla \psi_S(\mathbf{r})|^2 + |V(\mathbf{r})| |\psi_S(\mathbf{r})|^2) d\mathbf{r}.$$

Then  $\mathbb{D}$  is a metric space by the metric

$$r(\psi_S, \psi'_S) = \|\psi'_S - \psi_S\|$$

defined by the norm in the above .

Here  $\mathcal{D} = \mathcal{D}(S)$  is a space of all  $C^\infty$ -functions with compact support in  $S$ . Then we assume that  $\mathcal{D}$  is dense in  $\mathbb{D}$ .

Then  $J_S[\psi_S]$  is a continuous functional on  $\mathbb{D}$ .

Now we study the following local variational problem.

**Problem II (local variational problem)** We use the notation in the above. Then determine the  $L_{\text{loc}}^2$ -density  $\psi$  so that, for any compact set  $S$  which is not a null-set,  $\psi_S$  is a stationary function of the local energy functional  $J_S[\psi_S]$  defined on  $\mathbb{D}$ .

Now we put

$$I_S[\psi_S] = \int_S \left( \sum_{i=1}^n \frac{\hbar^2}{2m_i} \left| \frac{\partial \psi_S(\mathbf{r})}{\partial x_i} \right|^2 + V(\mathbf{r}) |\psi_S(\mathbf{r})|^2 \right) d\mathbf{r},$$

$$K_S[\psi_S] = \int_S |\psi_S(\mathbf{r})|^2 d\mathbf{r}.$$



Then we have

$$J_S[\psi_S] = \frac{I_S[\psi_S]}{K_S[\psi_S]}.$$

Then assume that we have a solution  $\psi$  of the local variational problem in the above. Namely we assume that we have a real number  $\mathcal{E}$  and an  $L_{\text{loc}}^2$ -function  $\psi$  which is not identically zero so that, for any compact set  $S$  in  $\mathbf{R}^n$  which is not a null-set and  $\psi_S = \psi\chi_S$ , we have either one of the following (1), (2) :

- (I)  $K_S[\psi_S] \neq 0$ , and,  $J_S[\psi_S] = \mathcal{E}$ .  
 (II)  $K_S[\psi_S] = 0$ .

Since the case (II) is evident, we consider the case (I).

Then, for a sufficiently small real parameter  $\varepsilon$ , we have, for any  $\varphi \in \mathbb{D}$ ,

$$\frac{d}{d\varepsilon}(J_S[\psi_S + \varepsilon\varphi])|_{\varepsilon=0} = 0, \quad (1)$$

$$\frac{d}{d\varepsilon}(J_S[\psi_S + i\varepsilon\varphi])|_{\varepsilon=0} = 0. \quad (2)$$

Now we put

$$I_S[\varphi, \psi_S] = \int_S \left( \sum_{i=1}^n \frac{\hbar^2}{2m_i} \frac{\overline{\partial\varphi(\mathbf{r})}}{\partial x_i} \frac{\partial\psi_S(\mathbf{r})}{\partial x_i} + V(\mathbf{r})\overline{\varphi(\mathbf{r})}\psi_S(\mathbf{r}) \right) d\mathbf{r},$$

$$K_S[\varphi, \psi_S] = \int_S \overline{\varphi(\mathbf{r})}\psi_S(\mathbf{r}) d\mathbf{r}.$$

Here  $\overline{\varphi(\mathbf{r})}$  denotes the complex conjugate of  $\varphi(\mathbf{r})$ .

Then we have

$$\begin{aligned} \frac{d}{d\varepsilon} J_S[\psi_S + \varepsilon\varphi] &= \frac{d}{d\varepsilon} \left( \frac{I_S[\psi_S + \varepsilon\varphi]}{K_S[\psi_S + \varepsilon\varphi]} \right) \\ &= \frac{\frac{d}{d\varepsilon}(I_S[\psi_S + \varepsilon\varphi])K_S[\psi_S + \varepsilon\varphi] - I_S[\psi_S + \varepsilon\varphi] \frac{d}{d\varepsilon}(K_S[\psi_S + \varepsilon\varphi])}{K_S[\psi_S + \varepsilon\varphi]^2}. \end{aligned}$$

Therefore we have

$$\frac{d}{d\varepsilon}(I_S[\psi_S + \varepsilon\varphi])|_{\varepsilon=0} = 2\text{Re } I_S[\varphi, \psi_S],$$

$$\frac{d}{d\varepsilon}(K_S[\psi_S + \varepsilon\varphi])|_{\varepsilon=0} = 2\text{Re } K_S[\varphi, \psi_S].$$

Here  $\text{Re } \alpha$  denotes the real part of a complex number  $\alpha$ .

Then we have

$$\frac{d}{d\varepsilon}(J_S[\psi_S + \varepsilon\varphi])|_{\varepsilon=0} = \frac{2\operatorname{Re} I_S[\varphi, \psi_S]}{K_S[\psi_S]} - \frac{2I_S[\psi_S]\operatorname{Re} K_S[\varphi, \psi_S]}{K_S[\psi_S]^2} = 0$$

by virtue of the formula (1).

Similarly, we have

$$\frac{d}{d\varepsilon}(J_S[\psi_S + i\varepsilon\varphi])|_{\varepsilon=0} = \frac{2\operatorname{Im} I_S[\varphi, \psi_S]}{K_S[\psi_S]} - \frac{2I_S[\psi_S]\operatorname{Im} K_S[\varphi, \psi_S]}{K_S[\psi_S]^2} = 0$$

by virtue of the formula (2).

Here  $\operatorname{Im} \alpha$  denotes the imaginary part of a complex number  $\alpha$ .

Hence we have

$$\frac{I_S[\varphi, \psi_S]}{K_S[\psi_S]} - \frac{I_S[\psi_S]K_S[\varphi, \psi_S]}{K_S[\psi_S]^2} = 0.$$

Then we have

$$J_S[\psi_S] = \frac{I_S[\psi_S]}{K_S[\psi_S]} = \mathcal{E}.$$

Therefore we have

$$I_S[\varphi, \psi_S] - \mathcal{E}K_S[\varphi, \psi_S] = 0.$$

Hence we have

$$\begin{aligned} & \int_S \left( \sum_{i=1}^n \frac{\hbar^2}{2m_i} \frac{\overline{\partial\varphi(\mathbf{r})}}{\partial x_i} \frac{\partial\psi_S(\mathbf{r})}{\partial x_i} \right) d\mathbf{r} \\ & + \int_S V(\mathbf{r})\overline{\varphi(\mathbf{r})}\psi_S(\mathbf{r})d\mathbf{r} - \mathcal{E} \int_S \overline{\varphi(\mathbf{r})}\psi_S(\mathbf{r})d\mathbf{r} = 0. \end{aligned}$$

By applying Plancherel's equality twice in the first term of this equality, we have

$$\left( \varphi, - \sum_{i=1}^n \frac{\hbar^2}{2m_i} \frac{\partial^2\psi_S}{\partial x_i^2} + V\psi_S - \mathcal{E}\psi_S \right)_S = 0.$$

Here  $(\cdot, \cdot)_S$  denotes the inner product in  $L^2(S)$ .

Then, because  $\varphi$  is an arbitrary element in  $\mathcal{D}$ , we have

$$- \sum_{i=1}^n \frac{\hbar^2}{2m_i} \frac{\partial^2\psi_S}{\partial x_i^2} + V\psi_S = \mathcal{E}\psi_S, \quad (\mathbf{r} \in S).$$

Thereby, because  $S$  is arbitrary, we have the differential equation

$$- \sum_{i=1}^n \frac{\hbar^2}{2m_i} \frac{\partial^2\psi}{\partial x_i^2} + V\psi = \mathcal{E}\psi, \quad (\mathbf{r} \in \mathbf{R}^n).$$

This is the **Euler differential equation** of the local variational problem. This is nothing else but the **Schrödinger equation** of the physical system considered here.

When we have the  $L^2_{\text{loc}}$ -density  $\psi$  which is not identically zero for the generalized eigenvalue problem for the Schrödinger operator,  $\mathcal{E}$  and  $\psi$  are said to be the **generalized eigenvalue** and the **generalized eigenfunction** of this Schrödinger operator  $H$  respectively. Especially,  $\psi$  is said to be the generalized eigenfunction belonging to the generalized eigenvalue  $\mathcal{E}$ .

This Schrödinger equation is the necessary condition in order that there exists a solution of this local variational problem. But, for the concrete physical system, we can prove the completeness of the system of generalized eigenfunctions of this generalized eigenvalue problem. Then, because we can completely determine the  $L^2$ -density of the total physical system by the generalized eigenfunction expansion, we can completely solve the Schrödinger equation.

In this sense, we can obtain the information of the natural probability distribution state of the physical system by solving the Schrödinger equation obtained here.

## 8 Solutions of periodic variational problems

In this section, we study the solutions of the periodic variational problems in order to derive the Schrödinger equations of the physical systems of the systems of micro-particles moving periodically. For the precise, we refer to Ito [12], section 9.1.

The Hamiltonian  $H$  appeared in the Schrödinger equation which describes the natural statistical phenomena of the physical system considered here has, generally, the form

$$H = - \sum_{i=1}^n \frac{\hbar^2}{2m_i} \frac{\partial^2}{\partial x_i^2} + V.$$

Here,  $m_i$ , ( $1 \leq i \leq n$ ) denote the masses of the micro-particles. The values of  $m_i$  corresponding to one micro-particle are the same.  $V$  denotes the potential which satisfies the periodic boundary conditions.

We call this operator  $H$  the **Hamiltonian operator**. In other word, we also call this the **Schrödinger operator**.

Let  $\mathbf{R}^n$  be the  $n$ -dimensional space. Here we assume  $n \geq 1$ . Put  $D = [-a, a]^n$  where  $a > 0$ .

Now we consider one physical system  $\Omega = \Omega(\mathcal{B}, P)$ . Mathematically, we consider that this is a probability space. Its elementary event  $\rho$  is one system of micro-particles which move periodically in  $D$ . Its position variable is  $\mathbf{r} = \mathbf{r}(\rho) = {}^t(x_1(\rho), x_2(\rho), \dots, x_n(\rho))$  and its momentum variable is  $\mathbf{p} = \mathbf{p}(\rho) = {}^t(p_1(\rho), p_2(\rho), \dots, p_n(\rho))$ .

We consider that the variable  $\mathbf{r}$  moves in  $D$  periodically and the variable  $\mathbf{p}$  moves in its dual space  $\mathbf{P}_n$  which is the countable set of  $n$ -column vectors whose components are integers.

Then, by virtue of the law II in Ito [12], section 9.1, the  $L^2$ -density  $\psi(\mathbf{r})$  determines the natural probability distribution law of the position variable  $\mathbf{r}$  and its Fourier coefficients  $\hat{\psi}(\mathbf{p})$  determines the natural probability distribution law of the momentum variable  $\mathbf{p}$ .

We assume that the potential  $V(\mathbf{r})$  is a real-valued measurable function on  $D$  which satisfies the periodic boundary conditions

$$V(\mathbf{r})|_{x_j=-a} = V(\mathbf{r})|_{x_j=a}, \quad (\mathbf{r} \in D, j = 1, 2, \dots, n).$$

Then we define the **energy functional**  $J[\psi]$  of  $L^2$ -density  $\psi(\mathbf{r})$  by the relation

$$J[\psi] = \int_D \left( \sum_{i=1}^n \frac{\hbar^2}{2m_i} \left| \frac{\partial \psi(\mathbf{r})}{\partial x_i} \right|^2 + V(\mathbf{r})|\psi(\mathbf{r})|^2 \right) d\mathbf{r}.$$

Here the integral denotes the Lebesgue integral on the interval  $D$ .

In this section, the partial derivatives of  $L^2$ -functions are defined in the sense of  $L^2$ -convergence. As for the precise, we refer to Ito [29], [34].

The domain of  $J[\psi]$  is the Hilbert space of all  $L^2$ -functions  $\psi$  given by the relation

$$\mathbb{D} = \left\{ \psi \in L^2; \int_D |\nabla \psi(\mathbf{r})|^2 d\mathbf{r} < \infty, \right. \\ \left. \int_D |V(\mathbf{r})||\psi(\mathbf{r})|^2 d\mathbf{r} < \infty \right\}$$

Here  $\nabla = \nabla_{\mathbf{r}}$  denotes the gradient operator.

$\mathbb{D}$  is the metric space with the metric

$$r(\psi, \psi') = \|\psi' - \psi\|$$

defined by the following norm

$$\|\psi\|^2 = \int_D (|\psi(\mathbf{r})|^2 + |\nabla \psi(\mathbf{r})|^2 + |V(\mathbf{r})||\psi(\mathbf{r})|^2) d\mathbf{r}.$$

Now we assume that  $\mathcal{D} = \mathcal{D}([-a, a]^n)$  is the space of all  $C^\infty$ -functions with compact support in  $D = [-a, a]^n$  and  $\mathcal{D}$  is dense in  $\mathbb{D}$ .

$J[\psi]$  is the continuous functional on  $\mathbb{D}$ .

Then we study the periodic variational problem in the following.

**Problem I (periodic variational problem)** We use the notation in the above. Then determine the stationary function  $\psi$  of the energy functional  $J[\psi]$  defined on  $\mathbb{D}$ . Here we assume that  $\psi \in \mathbb{D}$  satisfies the condition

$$\int_D |\psi(\mathbf{r})|^2 d\mathbf{r} = 1$$

and the periodic boundary conditions

$$\psi(\mathbf{r})|_{x_j=-a} = \psi(\mathbf{r})|_{x_j=a}, \quad (\mathbf{r} \in D, j = 1, 2, \dots, n).$$

Now, if we put

$$K[\psi] = \int_D |\psi(\mathbf{r})|^2 d\mathbf{r},$$

the periodic variational problem I in the above is the stationary value problem of  $J[\psi]$  under the condition

$$K[\psi] = 1.$$

Therefore we determine the stationary function using the Lagrange's method of indeterminate coefficients.

$\mathcal{E}$  being a Lagrange's indeterminate coefficient, we put

$$I[\psi] = J[\psi] - \mathcal{E}(K[\psi] - 1).$$

Then the conditional stationary value problem in the above is equivalent to the stationary value problem of  $I[\psi]$ .

Now, assume that we have a solution  $\psi$  of the conditional stationary problem in the above. Then this  $\psi$  is the stationary value problem of  $I[\psi]$ .

Then,  $\varepsilon$  being a sufficiently small real parameter, we have

$$\frac{d}{d\varepsilon}(I[\psi + \varepsilon\varphi])|_{\varepsilon=0} = 0, \quad (1)$$

$$\frac{d}{d\varepsilon}(I[\psi + i\varepsilon\varphi])|_{\varepsilon=0} = 0 \quad (2)$$

for any  $\varphi \in \mathbb{D}$ .

Then, by the formulas (1), (2), we have the equality

$$\sum_{i=1}^n \frac{\hbar^2}{2m_i} \left( \frac{\partial\varphi}{\partial x_i}, \frac{\partial\psi}{\partial x_i} \right) + (\varphi, V\psi) - (\varphi, \mathcal{E}\psi) = 0.$$

Here  $(\cdot, \cdot)$  denotes the inner product in  $L^2$ .

Using Plancherel's equality twice in the first term in this formula, we have the equality

$$\left( \varphi, - \sum_{i=1}^n \frac{\hbar^2}{2m_i} \frac{\partial^2\psi}{\partial x_i^2} + V\psi - \mathcal{E}\psi \right) = 0.$$

Because this formula holds for any  $\varphi \in \mathcal{D}$ , we have

$$- \sum_{i=1}^n \frac{\hbar^2}{2m_i} \frac{\partial^2\psi}{\partial x_i^2} + V\psi = \mathcal{E}\psi. \quad (3)$$

When we have a solution  $\psi \in \mathbb{D}$  which is not identically zero for the eigenvalue problem (3), we say that  $\mathcal{E}$  and  $\psi$  are the **eigenvalue** and the **eigenfunction** of the Schrödinger operator

$$H = - \sum_{i=1}^n \frac{\hbar^2}{2m_i} \frac{\partial^2}{\partial x_i^2} + V$$

respectively. Especially,  $\psi$  is the eigenfunction belonging to the eigenvalue  $\mathcal{E}$ .

This is the **Euler differential equation** for the conditional variational problem. We call this the **Schrödinger equation**.

This Schrödinger equation is the necessary condition in order for the existence of the solution of the periodic variational problem I in the above. For the concrete physical system, we can prove the completeness of the system of eigenfunctions of this eigenvalue problem.

Then, because we can determine the  $L^2$ -density for the total physical system completely by the eigenfunction expansion, we can solve this Schrödinger equation completely.

In this sense, by solving the Schrödinger equation obtained here, we can obtain the information on the natural probability distribution state of the physical system considered here.

## 9 Derivation of Schrödinger equation (1)

In this section, we study the derivation of Schrödinger equation using the variational principle. As for this, we refer to Ito [13]~[20], [22], [24], Ito-Kayama [1], [2], Ito-Kayama-Kamoshita [1], Ito-Uddin [1].

Let a probability space  $\Omega = \Omega(\mathcal{B}, P)$  be a certain physical system. An elementary event  $\rho$  in  $\Omega$  is a system of micro-particles as a combined system of some micro-particles. Then, let  $\mathbf{r} = \mathbf{r}(\rho) = {}^t(x_1(\rho), x_2(\rho), \dots, x_n(\rho))$  be the position variable of a system of micro-particles and  $\mathbf{p} = \mathbf{p}(\rho) = {}^t(p_1(\rho), p_2(\rho), \dots, p_n(\rho))$  be its momentum variable.

We assume that the position variable  $\mathbf{r}$  moves in the space  $\mathbf{R}^n$  and the momentum variable  $\mathbf{p}$  moves in the space  $\mathbf{R}^n$ .

Then, by virtue of Law II in section 2, an  $L^2$ -density  $\psi(\mathbf{r})$  determines the natural probability distribution law of the position variable  $\mathbf{r}$  and its Fourier transform  $\hat{\psi}(\mathbf{p})$  determines the natural probability distribution law of the momentum variable  $\mathbf{p}$ .

The total energy of each system of micro-particles, which is determined by the classical dynamics, has its value

$$\sum_{i=1}^n \frac{1}{2m_i} p_i(\rho)^2 + V(\mathbf{r}(\rho)).$$

Here the first term is the mechanical energy of the system of micro-particles and second term is the potential energy. There,  $m_i$  is the mass of a micro-particle.  $m_i$  has the same value for the one micro-particle. Thus, because one particle has  $d$  components of the momentum variable,  $d$  components of the momentum variable correspond to one value of  $m_i$ .

This energy variable is considered to be a natural random variable defined on the probability space  $\Omega$ .

In general, the random variable is a continuous random variable.

The expectation value of this energy variable, namely the energy expectation value is calculated in the following.

As a result, we have a Schrödinger operator

$$H = - \sum_{i=1}^n \frac{\hbar^2}{2m_i} \frac{\partial^2}{\partial x_i^2} + V.$$

Here we consider the case where the Schrödinger operator  $H$  has only the discrete spectrum. Then the energy expectation value is calculated by using the law II in section 2. Namely, when  $A$  and  $B$  are measurable sets in  $\mathbf{R}^n$ , we have the relations

$$P(\{\rho \in \Omega; \mathbf{r}(\rho) \in A\}) = \int_A |\psi(\mathbf{r})|^2 d\mathbf{r},$$

$$P(\{\rho \in \Omega; \mathbf{p}(\rho) \in B\}) = \int_B |\hat{\psi}(\mathbf{p})|^2 d\mathbf{p}.$$

Then the energy expectation value is equal to

$$\begin{aligned} E \left[ \sum_{i=1}^n \frac{1}{2m_i} p_i(\rho)^2 + V(\mathbf{r}(\rho)) \right] \\ = \int \left( \sum_{i=1}^n \frac{\hbar^2}{2m_i} |\psi_{x_i}(\mathbf{r})|^2 + V(\mathbf{r}) |\psi(\mathbf{r})|^2 \right) d\mathbf{r}. \end{aligned}$$

We denote this energy expectation value as follows:

$$J[\psi] = \int \left( \sum_{i=1}^n \frac{\hbar^2}{2m_i} |\psi_{x_i}(\mathbf{r})|^2 + V(\mathbf{r}) |\psi(\mathbf{r})|^2 \right) d\mathbf{r}.$$

We call this  $J[\psi]$  to be the **energy functional**.

In order to determine the natural probability distribution which is really realized among the admissible natural probability distributions, we postulate the variational principle I.

**Principle I (variational principle)** The stationary state of the physical system is realized as the state where the energy functional  $J[\psi]$  has its stationary value.

By using this principle, we choose the  $L^2$ -density which is realized physically in the real among the admissible  $L^2$ -densities for this physical system.

Therefor we consider the following variational problem I.

**Problem I (variational problem)** Determine the stationary function  $\psi$  of the energy functional  $J[\psi]$  under the condition

$$\int |\psi(\mathbf{r})|^2 d\mathbf{r} = 1.$$

Thus, we solve the variational problem I in section 6.

As the Euler's differential equation of the variational problem I, we obtain the Schrödinger equation

$$-\sum_{i=1}^n \frac{\hbar^2}{2m_i} \frac{\partial^2 \psi(\mathbf{r})}{\partial x_i^2} + V\psi(\mathbf{r}) = \mathcal{E}\psi(\mathbf{r}).$$

Here  $\mathcal{E}$  is Lagrange's indeterminate coefficient.

This Euler's differential equation is only a necessary condition for the stationary value problem.

But, in fact, if the obtained system of eigenfunctions satisfies the completeness condition, we can obtain the all information necessary for the physical system. Thus, the solution  $\psi$  of the variational problem I is obtained as the solution of the Schrödinger equation.

Now, the eigenfunctions  $\psi_m(\mathbf{r})$  and the eigenvalues  $\mathcal{E}_m$  satisfy the eigenvalue problem

$$-\sum_{i=1}^n \frac{\hbar^2}{2m_i} \frac{\partial^2 \psi_m(\mathbf{r})}{\partial x_i^2} + V(\mathbf{r})\psi_m(\mathbf{r}) = \mathcal{E}_m \psi_m(\mathbf{r}),$$

$$(m = 1, 2, 3, \dots).$$

Then we assume the system of eigenfunctions  $\{\psi_m(\mathbf{r})\}$  satisfies the orthonormality conditions and the completeness condition as follows.

(1) **(orthonormality condition).** We have the relations

$$\int \overline{\psi_j(\mathbf{r})} \psi_k(\mathbf{r}) d\mathbf{r} = \delta_{jk}, \quad (j, k = 1, 2, 3, \dots).$$

Here  $\delta_{jk}$  denotes the Kronecker's symbol and the integral means the Lebesgue integral on the space  $\mathbf{R}^n$ .

(2) **(completeness condition).** We have the relation

$$\sum_{m=1}^{\infty} \overline{\psi_m(\mathbf{r}')} \psi_m(\mathbf{r}) = \delta(\mathbf{r}' - \mathbf{r}), \quad (\mathbf{r}, \mathbf{r}' \in \mathbf{R}^n).$$



Here  $\delta(\mathbf{r}' - \mathbf{r})$  denotes the Dirac's measure.

Then, for any  $L^2$ -density  $\psi(\mathbf{r})$ , we have the eigenfunction expansion

$$\psi(\mathbf{r}) = \sum_{m=1}^{\infty} c_m \psi_m(\mathbf{r}),$$

$$c_m = \int \overline{\psi_m(\mathbf{r})} \psi(\mathbf{r}) d\mathbf{r}, \quad (m = 1, 2, 3, \dots).$$

Then, by the inverse process of the separation of variables, we derive the time-evolving Schrödinger equation.

At first, we consider the function

$$\psi_m(\mathbf{r}, t) = \psi_m(\mathbf{r}) \exp \left[ -i \frac{\mathcal{E}_m}{\hbar} t \right].$$

This satisfies the equation

$$i\hbar \frac{\partial \psi_m(\mathbf{r}, t)}{\partial t} = \mathcal{E}_m \psi_m(\mathbf{r}) \exp \left[ -i \frac{\mathcal{E}_m}{\hbar} t \right].$$

Here, for the Schrödinger operator  $H$ , we have the equations

$$H\psi_m(\mathbf{r}) = \mathcal{E}_m \psi_m(\mathbf{r}), \quad (m = 1, 2, 3, \dots).$$

Hence we have the equation

$$i\hbar \frac{\partial \psi_m(\mathbf{r}, t)}{\partial t} = H\psi_m(\mathbf{r}, t).$$

Now, by using the Fourier type coefficients  $\{c_m\}$  of the initial condition  $\psi(\mathbf{r})$ , we put

$$\psi(\mathbf{r}, t) = \sum_{m=1}^{\infty} c_m \psi_m(\mathbf{r}, t).$$

Then we have the relation

$$i\hbar \frac{\partial \psi(\mathbf{r}, t)}{\partial t} = H\psi(\mathbf{r}, t).$$

Namely, we have the solution  $\psi(\mathbf{r}, t)$  of the equation

$$i\hbar \frac{\partial \psi(\mathbf{r}, t)}{\partial t} = - \sum_{i=1}^n \frac{\hbar^2}{2m_i} \frac{\partial^2 \psi(\mathbf{r}, t)}{\partial x_i^2} + V(\mathbf{r})\psi(\mathbf{r}, t).$$

This is the time-evolving Schrödinger equation for the physical system considered here.

## 10 Derivation of Schrödinger equation (2)

In this section, we derive the Schrödinger equation by using the local variational principle. Namely we derive the Schrödinger equation in the case where the Schrödinger operator has the continuous spectrum. As for this, we refer to Ito [13]~[20], [22], [24] and Ito-Uddin [2].

In this case, in general, we consider the generalized eigenfunctions in  $L^2_{\text{loc}}$  of the Schrödinger operator in stead of the eigenfunctions in  $L^2$ .

In order to study this case, we must consider the state of the generalized natural probability distribution in stead of the physical state postulated in Law II. Therefore we study the problem in the frame of law I', law II' and law III' in section 3.

Then, by virtue of Law II',  $L^2_{\text{loc}}$ -density  $\psi(\mathbf{r})$  determines the generalized natural probability distribution law of the position variable  $\mathbf{r}$  and its Fourier transform  $\hat{\psi}(\mathbf{p})$  determines the generalized natural probability distribution law of the momentum variable  $\mathbf{p}$ .

Here the total energy of each system  $\rho$  of micro-particles is determined by virtue of the classical mechanics and has the value

$$\sum_{i=1}^n \frac{1}{2m_i} p_i(\rho)^2 + V(\mathbf{r}(\rho)).$$

This energy variable is considered to be a generalized natural random variable defined on a probability space  $\Omega'$  as the physical subsystem.

The local expectation value of this energy variable, namely the local energy expectation value is calculated by using law II'.

Namely, for an arbitrary compact set  $S$  in  $\mathbf{R}^n$  and two measurable sets  $A$  and  $B$  in  $\mathbf{R}^n$ , we use the relations

$$P(\{\rho \in \Omega; \mathbf{r}(\rho) \in A \cap S\}) = \frac{\int_{A \cap S} |\psi_S(\mathbf{r})|^2 d\mathbf{r}}{\int_S |\psi_S(\mathbf{r})|^2 d\mathbf{r}}$$

and

$$P(\{\rho \in \Omega; \mathbf{r}(\rho) \in S, \mathbf{p}(\rho) \in B\}) = \frac{\int_B |\hat{\psi}_S(\mathbf{p})|^2 d\mathbf{p}}{\int |\hat{\psi}_S(\mathbf{p})|^2 d\mathbf{p}}.$$

Then we have the local energy expectation value  $\bar{E}_S$  as follows :

$$\bar{E}_S = E_S \left[ \sum_{i=1}^n \frac{1}{2m_i} p_i(\rho)^2 + V(\mathbf{r}(\rho)) \right]$$

$$= \frac{\int_S \left( \sum_{i=1}^n \frac{\hbar^2}{2m_i} \left| \frac{\partial \psi_S(\mathbf{r})}{\partial x_i} \right|^2 + V(\mathbf{r}) |\psi_S(\mathbf{r})|^2 \right) d\mathbf{r}}{\int_S |\psi_S(\mathbf{r})|^2 d\mathbf{r}}.$$

Here we denote this local energy expectation value  $J_S[\psi_S]$  as follows :

$$J_S[\psi_S] = \frac{\int_S \left( \sum_{i=1}^n \frac{\hbar^2}{2m_i} \left| \frac{\partial \psi_S(\mathbf{r})}{\partial x_i} \right|^2 + V(\mathbf{r}) |\psi_S(\mathbf{r})|^2 \right) d\mathbf{r}}{\int_S |\psi_S(\mathbf{r})|^2 d\mathbf{r}}.$$

We call this  $J_S[\psi_S]$  to be the **local energy functional**.

Here we postulate the following principle.

**Principle II (local variational principle).** In the case where the Schrödinger operator of the physical system has the continuous spectrum, its stationary state is realized as the state which takes the stationary value of the energy expectation value of the physical system considered locally.

By using this principle, we choose the  $L^2_{\text{loc}}$ -density which is realized physically in the real among the admissible  $L^2$ -densities for this physical system.

Therefore we consider the following problem II.

Here we consider the case where the continuous spectrum of the Schrödinger operator is a nonnegative real number for fixing the subject. For the concrete physical systems, the various cases are considered accordingly to the forms of the Schrödinger operators.

**Problem II (local variational problem)** Let  $\{K_j\}$  be an increasing sequence of exhausting compact sets in  $\mathbf{R}^n$  which are not null-sets.

Namely this satisfies the following conditions (i) and (ii) :

$$(i) \quad K_1 \subset K_2 \subset \cdots \subset K_j \subset \cdots \subset \mathbf{R}^n.$$

$$(ii) \quad \bigcup_{j=1}^{\infty} K_j = \mathbf{R}^n.$$

Then, for an arbitrary non-negative real number  $\mathcal{E} \geq 0$ , determine the locally square integrable function  $\psi^{(\mathcal{E})}(\mathbf{r}) (\neq 0)$  so that the following conditions (1)~(5) are satisfied :

$$(1) \quad \psi^{(\mathcal{E})}|_{K_j} = \psi_j, \quad (j = 1, 2, 3, \cdots).$$

$$(2) \quad \psi_{j+1}|_{K_j} = \psi_j, \quad (j = 1, 2, 3, \cdots).$$

(3) For  $j = 1, 2, 3, \dots$ , we have one of the conditions (a), (b) in the following :

(a) The functional

$$J_j[\psi_j] = \frac{\int_{K_j} \left( \sum_{i=1}^n \frac{\hbar^2}{2m_i} \left| \frac{\partial \psi_j(\mathbf{r})}{\partial x_i} \right|^2 + V(\mathbf{r}) |\psi_j(\mathbf{r})|^2 \right) d\mathbf{r}}{\int_{K_j} |\psi_j(\mathbf{r})|^2 d\mathbf{r}}$$

has its stationary value.

(b)  $\psi_j = 0$ .

$$(4) \int \overline{\psi^{(\mathcal{E}')}(r)} \psi^{(\mathcal{E})}(r) dr = \delta(\mathcal{E}' - \mathcal{E}), \quad (\mathcal{E}', \mathcal{E} \geq 0).$$

Here  $\delta(\mathcal{E})$  denotes the Dirac measure.

$$(5) \int_0^\infty \overline{\psi^{(\mathcal{E})}(r')} \psi^{(\mathcal{E})}(r) d\mathcal{E} = \delta(r' - r), \quad (r, r' \in \mathbf{R}^n).$$

Solving the local variational problem, we have the Schrödinger equation

$$-\sum_{i=1}^n \frac{\hbar^2}{2m_i} \frac{\partial^2 \psi_j}{\partial x_i^2} + V(\mathbf{r}) \psi_j(\mathbf{r}) = \mathcal{E} \psi_j(\mathbf{r}),$$

$$(\mathbf{r} \in K_j; j = 1, 2, 3, \dots)$$

as the Euler's differential equation. Here  $\mathcal{E}$  is a Lagrange's indeterminate coefficient.

Eventhough the Euler's differential equation obtained here is only a necessary condition for the stationary value problem, all information necessary for the physical system is obtained if the system of generalized eigenfunctions obtained here satisfies the completeness condition (5). Then we obtain the  $L_{loc}^2$ -density  $\psi^{(\mathcal{E})}(\mathbf{r})$  which satisfies the conditions (1)~(3) in the problem II and satisfies

$$\psi^{(\mathcal{E})}(\mathbf{r}) = \psi_j(\mathbf{r}), \quad (\mathbf{r} \in K_j, j = 1, 2, 3, \dots)$$

for a certain  $\mathcal{E} \geq 0$ . Here  $\psi^{(\mathcal{E})}(\mathbf{r})$  satisfies the Schrödinger equation

$$-\sum_{i=1}^n \frac{\hbar^2}{2m_i} \frac{\partial^2 \psi^{(\mathcal{E})}(\mathbf{r})}{\partial x_i^2} + V(\mathbf{r}) \psi^{(\mathcal{E})}(\mathbf{r}) = \mathcal{E} \psi^{(\mathcal{E})}(\mathbf{r}), \quad (\mathbf{r} \in \mathbf{R}^n).$$

By virtue of the general expansion theorem, we define  $c(\mathcal{E})$  by the relation

$$c(\mathcal{E}) = \int \overline{\psi^{(\mathcal{E})}(\mathbf{r})} \psi(\mathbf{r}) d\mathbf{r}$$

for any  $L^2$ -density  $\psi(\mathbf{r})$ , we have

$$\psi(\mathbf{r}) = \int_0^\infty c(\mathcal{E})\psi^{(\mathcal{E})}d\mathcal{E}.$$

Here, we use the inverse process of the method of separation of variables. At first, we consider the function

$$\psi^{(\mathcal{E})}(\mathbf{r}, t) = \psi^{(\mathcal{E})}(\mathbf{r}) \exp \left[ -i\frac{\mathcal{E}}{\hbar}t \right].$$

Differentiating this function with respect to  $t$ , we have

$$i\hbar \frac{\partial \psi^{(\mathcal{E})}(\mathbf{r}, t)}{\partial t} = \mathcal{E}\psi^{(\mathcal{E})}(\mathbf{r}) \exp \left[ -i\frac{\mathcal{E}}{\hbar}t \right].$$

Here we represent the Schrödinger operator  $H$  for the stationary state by the relation

$$H = - \sum_{i=1}^n \frac{\hbar^2}{2m_i} \frac{\partial^2}{\partial x_i^2} + V(\mathbf{r}).$$

Then we have

$$H\psi^{(\mathcal{E})}(\mathbf{r}) = \mathcal{E}\psi^{(\mathcal{E})}(\mathbf{r}).$$

Hence we have

$$i\hbar \frac{\partial \psi^{(\mathcal{E})}(\mathbf{r}, t)}{\partial t} = \{ H\psi^{(\mathcal{E})}(\mathbf{r}) \} \exp \left[ -i\frac{\mathcal{E}}{\hbar}t \right] = H\psi^{(\mathcal{E})}(\mathbf{r}, t).$$

Therefore, if we put

$$\psi(\mathbf{r}, t) = \int_0^\infty c(\mathcal{E})\psi^{(\mathcal{E})}(\mathbf{r}, t)d\mathcal{E},$$

we have

$$i\hbar \frac{\partial \psi(\mathbf{r}, t)}{\partial t} = H\psi(\mathbf{r}, t)$$

Namely we have the solution  $\psi(\mathbf{r}, t)$  of the time-evolving Schrödinger equation

$$i\hbar \frac{\partial \psi(\mathbf{r}, t)}{\partial t} = - \sum_{i=1}^n \frac{\hbar^2}{2m_i} \frac{\partial^2 \psi(\mathbf{r}, t)}{\partial x_i^2} + V(\mathbf{r})\psi(\mathbf{r}, t).$$

Namely we have law III of section 3. Even in the case where the Schrödinger operator  $H$  has the continuous spectrum, the solution  $\psi(\mathbf{r}, t)$  of the Schrödinger equation which determines the physical state of the total physical system is an  $L^2$ -density at every time  $t$ .

By virtue of the conservation law of the probability, the time-evolving Schrödinger equation has no other form than the above.

By virtue of the laws of the natural statistical physics, the solution  $\psi$  of the Schrödinger equation is the  $L^2$ -density which determines the natural probability distribution of the position variable.

Therefore it is understood that the function  $\psi = \psi(\mathbf{r})$  is a function of real variables.

## 11 Derivation of Schrödinger equation (3)

In this section, we derive the Schrödinger equation for the system of micro-particles which are moving periodically by using the variational principle.

Let  $\Omega = \Omega(\mathcal{B}, P)$  be a physical system which satisfies laws in section 4.  $\Omega$  is a probability space.

An elementary event  $\rho$  in  $\Omega$  is a system of micro-particles which is a combined system of several micro-particles. These micro-particles move periodically.  $\mathbf{r} = \mathbf{r}(\rho) = {}^t(x_1(\rho), x_2(\rho), \dots, x_n(\rho))$  is the position variable of the system  $\rho$  of micro-particles and  $\mathbf{p} = \mathbf{p}(\rho) = {}^t(p_1(\rho), p_2(\rho) \cdots, p_n(\rho))$  is its momentum variable.

The position variable  $\mathbf{r}$  moves in the interval  $D = [-a, a]^n$  in the space  $\mathbf{R}^n$  and the momentum variable  $\mathbf{p}$  moves in the space  $\mathbf{P}_n$ .

Then, by virtue of law II, the  $L^2$ -density  $\psi(\mathbf{r})$  determines the natural probability distribution law of the position variable  $\mathbf{r}$  and its Fourier coefficients  $\psi(\mathbf{p})$  determine the natural probability distribution law of the momentum variable  $\mathbf{p}$ .

The total energy of each system of micro-particles is determined by the classical mechanics and its value is equal to

$$\sum_{i=1}^n \frac{1}{2m_i} p_i(\rho)^2 + V(\mathbf{r}(\rho)).$$

Here the first term denotes the kinetic energy of the system  $\rho$  of micro-particles and the second term denotes the potential energy. Here  $m_i$  denotes the mass of a micro-particle. The value of  $m_i$  corresponding to one micro-particle is the same. This energy variable is considered to be a natural random variable defined on the probability space  $\Omega$  which denotes the physical system.

In general, this is a continuous random variable.

We calculate the expectation value of this energy variable. We call this the energy expectation value.

In general, the Schrödinger operator  $H$  has the form

$$H = - \sum_{j=1}^n \frac{\hbar^2}{2m_j} \frac{\partial^2}{\partial x_j^2} + V$$

which will be known afterward.

**This operator  $H$  is said to be the Schrödinger operator.**

Here we assume the Schrödinger operator  $H$  has the discrete spectrum.

Then the energy expectation value is calculated by using law II in section 4 as follows. Namely, for a measurable set  $A$  in  $D$  and a subset  $B$  of  $\mathbf{P}_n$ , we calculate the energy expectation by the relation

$$\begin{aligned} E & \left[ \sum_{j=1}^n \frac{1}{2m_j} p_j(\rho)^2 + V(\mathbf{r}(\rho)) \right] \\ & = \int_D \left( \sum_{i=1}^n \frac{\hbar^2}{2m_i} |\psi_{x_i}(\mathbf{r})|^2 + V(\mathbf{r}) |\psi(\mathbf{r})|^2 \right) d\mathbf{r}. \end{aligned}$$

In this calculation, we use the Parseval's equality for the Fourier series.  $\psi_{x_i}$  denotes the partial  $L^2$ -derivative with respect to the variable  $x_i$  in the sense of  $L^2$ -convergence.

Here we put this energy expectation in the form

$$J[\psi] = \int_D \left( \sum_{i=1}^n \frac{\hbar^2}{2m_i} |\psi_{x_i}(\mathbf{r})|^2 + V(\mathbf{r}) |\psi(\mathbf{r})|^2 \right) d\mathbf{r}.$$

We call  $J[\psi]$  the **energy functional**

The domain  $\mathbb{D}$  of  $J[\psi]$  is the space of  $L^2$ -functions

$$\mathbb{D} = \left\{ \psi \in L^2; \int_D |\nabla \psi(\mathbf{r})|^2 d\mathbf{r} < \infty, \int_D |V(\mathbf{r})| |\psi(\mathbf{r})|^2 d\mathbf{r} < \infty \right\}.$$

The norm of  $\mathbb{D}$  is defined by the relation

$$\|\psi\|^2 = \int_D \left( |\psi(\mathbf{r})|^2 + |\nabla \psi(\mathbf{r})|^2 + |V(\mathbf{r})| |\psi(\mathbf{r})|^2 \right) d\mathbf{r}.$$

Here  $\mathcal{D} = \mathcal{D}([-a, a]^n)$  is defined to be the space of all  $C^\infty$ -functions with compact support in  $D = [-a, a]^n$ .

We assume that  $\mathcal{D}$  is dense in  $\mathbb{D}$ .  $J[\psi]$  is a continuous functional on  $\mathbb{D}$ .

In order to determine the natural statistical state realized really among the admissible natural statistical states, we postulate the principle I in the following.

**Principle I (variational principle)** The stationary state of the physical system is realized as the state where the energy functional of the physical system takes its stationary value.

We show that we can derive the Schrödinger equation by solving the variational problem in the following on the basis of the principle I,

**Problem I (variational problem)** Determine the stationary function  $\psi$  of the energy functional  $J[\psi]$  among the admissible  $L^2$ -densities  $\psi$ . Here we assume that  $\psi(\mathbf{r})$  is an  $L^2$ -density which satisfies the periodic boundary conditions :

$$\psi(\mathbf{r})|_{x_j=-a} = \psi(\mathbf{r})|_{x_j=a}, \quad (\mathbf{r} \in D, j = 1, 2, \dots, n).$$

We put

$$K[\psi] = \int_D |\psi(\mathbf{r})|^2 d\mathbf{r}.$$

Then the variational problem I in the above is the variational problem of  $J[\psi]$  under the condition

$$K[\psi] = 1.$$

$\mathcal{E}$  being a Lagrange's indeterminate coefficient, we put

$$I[\psi] = J[\psi] - \mathcal{E}(K[\psi] - 1).$$

Then the conditional stationary value problem in the above is equivalent to the stationary value problem for  $I[\psi]$ .

Now assume that we have a solutions  $\psi$  of the conditional stationary value problem in the above.

Then, by solving the stationary value problem for  $I[\psi]$ , we have the Schrödinger equation

$$-\sum_{i=1}^n \frac{\hbar^2}{2m_i} \frac{\partial^2 \psi}{\partial x_i^2} + V\psi = \mathcal{E}\psi.$$

Thus, by solving the conditional variational problem, we have the **Schrödinger equation** as the **Euler's differential equation**.

This Schrödinger equation is a necessary condition in order that we have a solution of the variational problem I in the above.

For a real physical system, we can prove the completeness condition of the solutions of this eigenvalue problem. Then, because we can determine the  $L^2$ -density completely for the total physical system by virtue of the eigenfunction expansion, we can solve the Schrödinger equation completely.

In this sense, by solving the Schrödinger equation obtained here, we can obtain the information concerning the natural statistical state of the physical system.

In general, there are many stationary states where the energy expectations are the stationary value in one physical system.

The  $L^2$ -density which is a stationary state is an eigenfunction of the Schrödinger equation in the above and the stationary value of its energy functional is the eigenvalue.



The physical subsystem whose natural probability distribution is determined by such a eigenfunction is said to be a proper physical subsystem.

Then the physical system considered here is the composite state of those proper physical subsystems.

Further the  $L^2$ -density which is the physical state of the total physical system is given by the eigenfunction expansion using the system of eigenfunctions. Then the energy expectation of each proper physical subsystem is equal to the eigenvalue corresponding to it.

For one system of micro-particles, the position variable is the quantity which moves continuously with time  $t$  and the momentum variable is the quantity which moves continuously with almost every time  $t$ .

Nevertheless, the position variable and the momentum variable of the systems of micro-particles composing the physical system are the quantities which depend randomly on every system of micro-particles at the definite time.

Now assume that the eigenfunction  $\psi_m(\mathbf{r})$  and the eigenvalue  $\mathcal{E}_m$  of the eigenvalue problem in the above satisfy the equations

$$-\sum_{i=1}^n \frac{\hbar^2}{2m_i} \frac{\partial^2 \psi_m(\mathbf{r})}{\partial x_i^2} + V(\mathbf{r})\psi_m(\mathbf{r}) = \mathcal{E}_m \psi_m(\mathbf{r}),$$

$$(\mathbf{r} \in D, m = 1, 2, 3, \dots).$$

Here we consider that the periodic boundary conditions are always satisfied and do not mention this fact in every case.

Then this system of eigenfunctions  $\{\psi_m(\mathbf{r})\}$  satisfies the orthonormality condition and the completeness condition in the following:

(1) **(orthonormality condition)** We have the relations

$$\int_D \overline{\psi_j(\mathbf{r})} \psi_k(\mathbf{r}) d\mathbf{r} = \delta_{j,k}, (j, k = 1, 2, 3, \dots).$$

Here  $\delta_{j,k}$  denotes the Kronecker's delta and the integral denotes the Lebesgue integral on the whole space  $D$ .

(2) **(completeness condition)**. We have the relations

$$\sum_{m=1}^{\infty} \overline{\psi_m(\mathbf{r}')} \psi_m(\mathbf{r}) = \delta(\mathbf{r}' - \mathbf{r}), (\mathbf{r}', \mathbf{r} \in D)$$

Here  $\delta(\mathbf{r}' - \mathbf{r})$  denotes the Dirac's measure.

Then, an arbitrary  $L^2$ -density  $\psi(\mathbf{r})$  has the eigenfunction expansion

$$\psi(\mathbf{r}) = \sum_{m=1}^{\infty} c_m \psi_m(\mathbf{r}),$$

$$c_m = \int_D \overline{\psi_m(\mathbf{r})} \psi(\mathbf{r}) d\mathbf{r}, \quad (m = 1, 2, 3, \dots)$$

Here we use the inverse process of the separation of variables and obtain the time-evolving Schrödinger equation

At first, we consider the function

$$\psi_m(\mathbf{r}, t) = \psi_m(\mathbf{r}) \exp \left[ -i \frac{\mathcal{E}_m}{\hbar} t \right].$$

By differentiating both sides with respect  $t$ , we have

$$i\hbar \frac{\partial \psi_m(\mathbf{r}, t)}{\partial t} = \mathcal{E}_m \psi_m(\mathbf{r}) \exp \left[ -i \frac{\mathcal{E}_m}{\hbar} t \right].$$

Here, putting the Schrödinger operator  $H$  of the physical system

$$H = - \sum_{i=1}^n \frac{\hbar^2}{2m_i} \frac{\partial^2}{\partial x_i^2} + V(\mathbf{r}),$$

we have

$$H\psi_m(\mathbf{r}) = \mathcal{E}_m \psi_m(\mathbf{r}), \quad (m = 1, 2, 3, \dots).$$

Hence we have

$$i\hbar \frac{\partial \psi_m(\mathbf{r}, t)}{\partial t} = H\psi_m(\mathbf{r}, t).$$

Here, by using the Fourier type coefficients  $\{c_m\}$  of the initial condition  $\psi(\mathbf{r})$ , we put

$$\psi(\mathbf{r}, t) = \sum_{m=1}^{\infty} c_m \psi_m(\mathbf{r}, t).$$

Then  $\psi(\mathbf{r}, t)$  satisfies the equation

$$i\hbar \frac{\partial \psi(\mathbf{r}, t)}{\partial t} = H\psi(\mathbf{r}, t).$$

Namely, we have the equation

$$i\hbar \frac{\partial \psi(\mathbf{r}, t)}{\partial t} = - \sum_{i=1}^n \frac{\hbar^2}{2m_i} \frac{\partial^2 \psi(\mathbf{r}, t)}{\partial x_i^2} + V(\mathbf{r})\psi(\mathbf{r}, t).$$

This is the time-evolving Schrödinger equation for the physical system considered here. Therefore we have the following theorem.

**Theorem** *Assume that the functions  $\psi(\mathbf{r})$  and  $\psi(\mathbf{r}, t)$  are given in the above of this theorem. Then,  $\psi(\mathbf{r}, t)$  is the solution of the initial-boundary value problem for the time-evolving Schrödinger equation*

$$i\hbar \frac{\partial \psi(\mathbf{r}, t)}{\partial t} = - \sum_{i=1}^n \frac{\hbar^2}{2m_i} \frac{\partial^2 \psi(\mathbf{r}, t)}{\partial x_i^2} + V(\mathbf{r})\psi(\mathbf{r}, t),$$

$$\psi(\mathbf{r}, 0) = \psi(\mathbf{r}), \quad (\mathbf{r} \in D), \quad (\text{Initial condition}),$$

$$\psi(\mathbf{r})|_{x_j=-a} = \psi(\mathbf{r})|_{x_j=a}, \quad \psi(\mathbf{r}, t)|_{x_j=-a} = \psi(\mathbf{r}, t)|_{x_j=a},$$

$$(\mathbf{r} \in D, 0 < t < \infty), \quad (j = 1, 2, \dots, n), \quad (\text{periodic boundary condition}).$$

## 12 Solutions of problems of natural statistical physics

Until now, the following problems are solved by using the “natural statistical physics” .

**(1) Laws(general).** We established the laws of natural statistical physics in the general form in the three cases. These are the renaming of the axioms of natural statistical physics or the axioms of new quantum theory. As for the precise, we refer to Ito [1], [5], [6], [8], [9], [13]~[16],[18], [20], [26], [27], [31].

In this paper, we give the final expression of these general laws of natural statistical physics

**(2) Solutions of the variational problems.** We derive the Schrödinger equation in the stationary state as Euler’s differential equation for the variational problem of the energy functional of the physical system. Thereby, we can succeed to derive the Schrödinger equation naturally and reasonably in the exact sense of mathematics. As for the precise, we refer to Ito [13], [14], [15], [16], [17].[18], [19], [20], [22], [26], Ito-Kayama[51], [52].

**(3) Derivation of the Schrödinger equation.** By solving the eigenvalue problem for the Schrödinger equation in the stationary states, we obtain the system of eigenfunctions of the Schrödinger operator.

By using the inverse process of separation of variables, we obtain the time-evolving Schrödinger equation. By using the solution of this time-evolving Schrödinger equation, we can obtain the mathematical informations of the natural statistical distribution of the position variable and the momentum variable of the physical system completely. As for the precise, we refer to Ito [5], [6], [13], [14], [15], [16], [18], [19], [20], [22], [26], [50], Ito-Kayama, [51], [52].

**(4) Harmonic oscillator.** We derive the Schrödinger equation of the system of harmonic oscillators and solve this equation. As for the precise, we refer to Ito [16].

**(5) Black body radiation and Planck's formula of radiation.** We study the problem of black body radiation and derive Planck's formula of radiation naturally and reasonably by using the theory of natural statistical physics. As for the precise, we refer to Ito [16] and [17], Ito-Kayama-Kamosita[1].

**(6) Specific heat of a solid.** We study the problem of the specific heat of a solid by using the theory of natural statistical physics, Thereby we succeeded in understanding the specific heat of a black body or a monatomic solid by using Einstein model and Debye model respectively. As for the precise, we refer to Ito [16], [28] and Ito-Uddin [54].

**(7) Specific heat of an ideal gas.** We study the problem of the specific heat of an ideal gas by using the theory of natural statistical physics. Thereby we succeeded in understanding the specific heat of an ideal gas naturally and reasonably. As for the precise, we refer to Ito [16] and Ito-Uddin [55].

**(8) Tunnel effect.** We study the phenomena of potential barrier by using the theory of natural statistical physics. Thereby we succeeded in understanding the tunnel effect naturally and reasonably. As for the precise, we refer to Ito [20], [25].

**(9) Conductor and electric current.** We study the phenomena of potential well by using the theory of natural statistical physics. Thereby we succeeded in understanding the phenomena of conductor and electric current and trapping effect naturally and reasonably. As for the precise, we refer to Ito [20], [38].

**(10) Double slit experiment.** We study the phenomena of double slit experiment by using the theory of natural statistical physics. Thereby we succeeded in understanding the phenomena of double slit experiment. We also study A. Tonomura's experiment of bi-prism of electron beam as an example of double slit experiment. Thereby we understand that the phenomena of double slit experiment are the natural statistical phenomena. This is the evidence of the reality of the theory of natural statistical physics. As for the precise, we refer to Ito [20], [49].

**(11) Spectrum of hydrogen atoms and Stability of hydrogen atoms.** We study the spectrum of hydrogen atoms and the stability of hydrogen atoms by using the theory of natural statistical physics. Thereby we prove the Bohr's law of the spectra of hydrogen atoms and the stability of hydrogen atoms. As for the precise we refer to Ito[20], [27], [39].

**(12) Angular momentum.** We study the angular momentum of hydrogen atoms by using the theory of natural statistical physics. Thereby we

obtain the expectation value of hydrogen atoms and atomic structure of hydrogen atoms. Especially we obtain the value of Bohr's radius. As for the precise, we refer to Ito[20], [24], [27], [37], [39].

## 13 Unsolved problems

From now on, the physics must be studied by using Newtonian mechanics, Maxwell electro-magnetic dynamics and natural statistical physics.

Especially we must study again the old studies of physics by using the theory of old "quantum mechanics."

Of course, there will be many physical phenomena which cannot be understood using those three physical theories. In order to understand these physical phenomena, it is expected to create the new physical theories.

The future problems of my study are the following:

- (1) Statistical thermodynamics
  - (i) phenomena of heat.
  - (ii) phenomena of light.
  - (iii) phenomena of ideal gas.
  - (iv) phenomena of specific heat.
  - (v) entropy
  - (vi) laws of thermodynamics.
- (2) physics of atoms.
  - (i) angular momentum and spin.
  - (ii) composition of angular momenta.
  - (iii) atomic structure.
- (3) physics of molecules.

## 14 Table of correspondence of new and old terminologies

In this section, we give the table of correspondence of new and old terminologies in the theory of natural statistical physics which is the renaming of new quantum theory.

**Example** new terminology(old terminologies), such as  
 · natural statistical physics (new quantum theory)

### << Table >>

- generalized natural random variable (generalized quantum random variable)
- generalized proper natural statistical state (generalized proper quantum state)
- generalized proper physical system (generalized proper quantum system)
- law of natural statistical physics (axiom of natural statistical physics or axiom of new quantum theory)
- $L^2$  natural random variable ( $L^2$  quantum random variable)
- natural expectation (quantum expectation)
- natural probability (quantum probability)
- natural probability density (quantum probability density)
- natural probability distribution (quantum probability distribution)
- natural statistical physics (new quantum theory)
- natural statistical state (quantum state)
- $n$ -th proper physical system ( $n$ -th proper quantum system)
- photon hypothesis (light quantum hypothesis)
- physical system (quantum system)
- proper natural statistical state (proper quantum state)
- proper physical system (proper quantum system)
- vector valued natural random variable (vector valued quantum random variable)

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