What are Happening in the Physics of Electrons, Atoms and Molecules? Physical Reality Revisited

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Abstract

In this paper, we study the fundamental principles of natural statistical physics, which is the renaming of new quantum theory and some concrete physical phenomena of electrons, atoms and molecules, which are understood by this new theory. Establishing my new theory, I succeeded in solving Einstein-Bohr's argument.

I also give the solution of Hilbert's 6th Problem.

Introduction

What does it mean that we understand some physical phenomena?

How can we understand the concrete physical phenomena?

In my theory, we give the answers for these questions in the cases of natural statistical phenomena.

My theory is not an interpretation of the physical phenomena.

My theory is the discovery of the natural law of the natural statistical physics.

Every particle in the nature has its proper mass and its proper electric charge. Then every particle is moving by the Newtonian equation of motion by the cause of Coulomb force approximately.

So that, every particle has the position, the momentum and the energy.

Generally speaking, different particles have different values of these physical variables.

In order to explain these phenomena, we usually use the probability space and the random variables in the theory of mathematics.

Then we consider the position variables and the momentum variables to be the random variables on the probability spaces as the physical systems of particles.

In the natural statistical physics, the characteristic property is that the probability distributions of these random variables are determined by L^2 -densities or L^2_{loc} -densities.

Namely, the probability distribution of the position variables of some physical system is determined by L^2 -density $\psi(r)$ and that of the momentum variables is determined by its Fourier transform $\hat{\psi}(p)$.

Using this principles, we get the Schrödinger equation of the physical system.

Using my theory, we can understand many natural statistical phenomena which are studied in the rest of this paper.

By using the solutions of Schrödinger equations as L^2 -densities, we can obtain the informations of the physical states of the considered physical systems completely.

1 What is the Physical Reality?

Here we remember the Einstein's question.

Einstein asked what is the physical reality.

After that, Einstein-Bohr's argument started and continued very long time.

But, I know now, they could not find its true solution at that time.

After all, Einstein stopped the argument. But he considered his problem from that time forward.

Nevertheless, he could not find the answer after all.

Now, I ask what is the physical reality once again.

I have very many questions in the old quantum theory.

These are the following problems of the old quantum theory.

What is the quantum?

What physical substance is the quantum?

Is the quantum a substance of only one kind?

I have not yet found the clear and evident definition of the concept of quantum in the old literatures.

What are the quantum system and the quantum state?

Namely, what physical system is a quantum system concretely?

What physical state of the concrete physical system is the quantum state?

What is the quantization?

Only by the quantization process as a mathematical process, why does the physical phenomena represented by the classical Hamiltonian change into the "quantum phenomena"?

Namely, does the mathematical process of calculation change the physical phenomena really?

Why are the Schrödinger equations fundamental equations in the quantum theory?

What is the wave function?

In the representation of wave function, what are the variables of position and momentum under the consideration of Heisenberg's uncertainty principle?

Can we determin the values of these variables concretely? If not so, how can we represent the Schrödinger equatin as the partial differential equation. Namely, can we differentiate the wave function by these ambiguous "variables"?

Why can we understand the "quantum phenomena" by the "probability interpretation" of the wave function?

Here what is the probability?

As for only one particle, can we consider the probability of the position?

Mathematically, we cannot consider the probability of the position of one particle.

In fact, we have not the probability space for the "quantum system" composed of only one particle.

We can speak about the probability of some probability event in the framework of the probability space.

Is it true the wave functions go through the square potential barrier?

Is a wave function a physical substance?

Is it true that one electron is a particle and a wave at the same time?

I know that the function is a mathematical concept but not a physical substance.

The function gives only the digital data by the correspondence of independent variables to its values in the theory of mathematics.

Namely, a wave function is not any particle.

What is the physical quantity?

What does it mean that the physical quantity is discrete?

Why does the Hermite operator correspond to the physical quantity as an observable?

Why is the eigenvalue of an Hermite operator the observed physical quantity?

Without using the physical principles and the physical laws, can we understand any physical phenomena?

What physical principles and what physical laws should we use for understanding the "quantum phenomena"?

Everything is wrapped in mystery.

2 Natural Statistical Physics

I have recently succeeded in clarifying the true meanings of the old quantum phenomena in the very new framework, namely in the theory of natural statistical physics by the completely different way.

Do you know what are happening in the physics of electrons, atoms and molecules? Here, I give the survey on the research on natural statistical physics until now.

At the time 1920's when the old quantum mechanics was discovered, many physicists and mathematicians in the world did not understand its true meaning. But they tried to understand the new mechanics and tried to understand "quantum phemonena" by using it.

80 years after, we know the mistake of the old quantum mechanics.

Now the theory of natural statistical physics, which is the renaming of the new quantum theory, has been established as the true theory for understanding the physical phenomena of electrons, atoms and molecules.

Schrödinger equation is established as the natural law on the same level as Newton's equation of motion and Maxwell's equation of electro-magnetic field.

Nevertheless, nobody now investigates the new theory except myself.

In this time, we make clear the known facts until now.

After all I succeeded in solving Einstein-Bohr's argument and giving the true answer. The known facts until now are the following:

- Natural Probability (renaming of Quantum Probability)
- 2 Axiom of Natural Statistical Physics (renaming of New Quantum Theory)

Here we give the solution of Hilbert's 6th Problem.

- 3 Derivation of Schrödinger Equations
- 4 Harmonic Oscillator
- 5 Black Body Radiation and Planck's Formula of Radiation
- 6 Specific Heat of Solid Matter
- 7 System of Free Particles
- 8 Specific Heat of Ideal Gas
- 9 Square Potential Barrier and Tunnel Effect
- 10 Potential Energy Well
- 11 Potential Energy Well of Infinite Depth
- 12 Experiment of Double Slits
- 13 Spectrum of Hydrogen Atoms
- 14 Philosophy of Natural Statistical Physics

Here we prove the stability of atoms and we show what are sound, heat and light.

3 Natural Probability

Let \mathbb{R}^n , $(n \geq 1)$ be the *n*-dimensional Euclidean space and the triplet $(\mathbb{R}^n, \mathcal{M}_n, d\mathbf{r})$ the space of Lebesgue measure. Let $L^2 = L^2(\mathbb{R}^n)$ be the Hilbert space of all square integrable functions on \mathbb{R}^n . $\|\cdot\|$ denotes the Hilbert norm in L^2 .

For $\psi \in L^2$, $(\|\psi\| = 1)$ and $A \in \mathcal{M}_n$, we put $\xi_A(r) = \xi(A; r) = \chi_A(r)\psi(r)$. Here $\chi_A(r)$ denotes the characteristic function of a measurable set A.

Here we put

$$\mu(A) = \|\xi_A\|^2 = \int_A |\psi(r)|^2 dr$$

Then the triplet $(\mathbf{R}^n, \mathcal{M}_n, \mu)$ becomes a probability space.

Definition 3.1 We use the above notation. We call the L^2 -valued set function $\xi_A = \chi_A \psi$ defined on \mathcal{M}_n an **orthogonal probability measure** defined on the probability space $(\mathbf{R}^n, \mathcal{M}_n, \mu)$. We call this a **natural probability** defined by the L^2 -density ψ , which is the renaming of a quantum probability.

Definition 3.2 Let $\Omega = \Omega(\mathcal{B}, P)$ be a probability space and $r = r(\omega)$ a vector valued function defined on Ω . Then $r = r(\omega)$ is said to be a vector valued natural random variable if the following conditions (i)~(iii) are satisfied:

- (i) For $A \in \mathcal{M}_n$, we have $\{\omega; \boldsymbol{r}(\omega) \in A\} \in \mathcal{B}$.
- (ii) For $A \in \mathcal{M}_n$, we have $\mu(A) = P(\{\omega; r(\omega) \in A\})$. Then the triplet $(\mathbf{R}^n, \mathcal{M}_n, \mu)$ is a probability space.
- (iii) μ is absolutely continuous with respect to the Lebesgue measure and there exists some L^2 -density $\psi(r)$ such that we have

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

Theorem 3.1 Let $r = r(\omega)$ is the same as in Definition 3.2. Let $\Phi(r)$ be a Lebesgue measurable function of r.

Then, for the expectation value $E[\Phi(r(\omega))]$ of the random variable $\Phi(r(\omega))$, we have the following:

$$E[\Phi(m{r}(\omega))] = \int \Phi(m{r}) |\psi(m{r})|^2 dm{r}.$$

This equality has the meaning when the integral on the right hand side converges absolutely.

4 Axiom of Natural Statistical Physics

As the axiom of natural statistical physics, we define the following: (1) physical system, (2) physical state and (3) motion of the physical system.

Axiom I (physical system) We define the physical system Ω to be the probability space $\Omega(\mathcal{B}, P)$. Here Ω is the ensemble of systems ρ of microparticles, \mathcal{B} is the σ -algebra of the family of subsets of Ω and P is the completely additive probability measure defined on \mathcal{B} .

Axiom II (physical state) We define the physical state of the physical system $\Omega = \Omega(\mathcal{B}, P)$ to be the states of the natural probability distributions of the position variables $\mathbf{r}(\rho)$ and the momentum variables $\mathbf{p}(\rho)$ of the systems ρ of microparticles.

- (II₁) The natural probability distribution of the position variables $r = r(\rho)$ is determined by an L^2 -density $\psi(r)$ defined on \mathbb{R}^n .
- (II₂) The natural probability distribution of the momentum variables $p = p(\rho)$ is determined by the Fourier transform $\hat{\psi}$ of ψ .

Here we put

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

(II₃) For a Lebesgue measurabale set A in \mathbb{R}^n , we have

$$P(\{
ho\in\Omega; oldsymbol{r}(
ho)\in A\})=\int_A |\psi(oldsymbol{r})|^2 doldsymbol{r}=\mu(A).$$

Thereby, we have a probability space $(\mathbf{R}^n, \mathcal{M}_n, \mu)$.

(II₄) For a Lebesgue measurable set B in R_n , we have

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

Thereby, we have a probability space $(\mathbf{R}_n, \mathcal{N}_n, \nu)$.

Axiom III (motion of the physical system) We define the motion of the physical system to be the time evolution of the L^2 -density $\psi(\mathbf{r},t)$ of a physical system depending on the time t.

The law of the motion of the physical system is described by a Schrödinger equation. The Schrödinger equation is represented in the form

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

The Schrödinger operator H is a self-adjoint operator on some Hilbert space.

In order that the solution $\psi(\mathbf{r},t)$ of the Schrödinger equation in Axiom III is an L^2 -density depending on time t, this L^2 -density must be a complex-valued real function depending on real variables \mathbf{r} and t.

For the L^2 -density $\psi(\mathbf{r},t)$ depending on time t, the conservation law of probability holds.

Therefore we see that the Schrödinger operator must be a self-adjoint operator and the Schrödinger equation must include the partial derived function of degree one with respect to time variable and must be only of the form in Axiom III.

In the principle of superposition, the complex phase of L^2 -density, which is a solution of the Schrödinger equation, plays an important role.

Therefore, we must determine the L^2 -density of the physical system up to its complex phase.

But, some physical data on the physical state of the physical system in the real do not depend such a complex phase and are known by virtue of the data only on the absolute value of the L^2 -density in many cases.

In cases where the Schrödinger operators have the continuous spectra, we need the generalized axiom of the natural statistical physics.

This is defined in the following.

Axiom I' ((generalized) proper physical system) The proper physical system Ω' or the generalized proper physical system Ω' is a probability subspace of the total physical system Ω . Namely this is a physical subsystem of Ω .

This satisfies the following Axiom III' and Axiom III'.

Axiom II' ((generalized) proper physical state)

- (1) In the case where the Schrödinger operator of the total physical system has only the discrete spectrum, the proper physical states of the proper physical system are determined by the eigenfunctions ψ of the Schrödinger operator in the same way as in Axiom II.
- (2) In the case where the Schrödinger operator of the total physical system has the continuous spectrum, the generalized proper physical states of the generalized proper physical system Ω' is determined by the generalized eigenfunctions ψ of the Schrödinger operator in the following (II'₁)~(II'₄).
- (II'₁) The generalized natural probability distribution of the position variables $r = r(\rho)$ is determined by an L^2_{loc} -function ψ defined on \mathbb{R}^n .
- (II'₂) The generalized natural probability distribution of the momentum variables $p = p(\rho)$ is determined by $\hat{\psi}$. Here $\hat{\psi}$ is the local Fourier transform of ψ . Namely, $\hat{\psi}$ is determined locally by the relation

$$\hat{\psi}_S(oldsymbol{p}) = (2\pi\hbar)^{-n/2} \int \psi_S(oldsymbol{r}) e^{-i(oldsymbol{p}\cdotoldsymbol{r})/\hbar} doldsymbol{r}.$$

Here we put $\psi_S(\mathbf{r}) = \psi(\mathbf{r})\chi_S(\mathbf{r})$, where S is a compact set in \mathbf{R}^n .

 (II'_3) For a Lebesgue measurable set A in \mathbb{R}^n , we have

$$P(\{
ho\in\Omega;m{r}(
ho)\in A\cap S\})=rac{\displaystyle\int_{A\cap S}|\psi_S(m{r})|^2dm{r}}{\displaystyle\int_S|\psi_S(m{r})|^2dm{r}}=\mu_S(A).$$

Thereby, we have a relative probability space $(\mathbf{R}^n, \mathcal{M}_n \cap S, \mu_S)$ determined by ψ_S .

 (II'_4) For a Lebesgue measurable set B in \mathbf{R}_n , we have

$$P(\{
ho\in\Omega; oldsymbol{r}(
ho)\in S, oldsymbol{p}(
ho)\in B\}) = rac{\displaystyle\int_{B}|\hat{\psi}_{S}(oldsymbol{p})|^{2}doldsymbol{p}}{\displaystyle\int|\hat{\psi}_{S}(oldsymbol{p})|^{2}doldsymbol{p}} =
u_{S}(B).$$

Thereby, we have a relative probability space $(R_n, \mathcal{N}_n, \nu_S)$ determined by $\hat{\psi}_S$.

By virtue of Axiom II', we see that the L_{loc}^2 -density $\psi(r)$ representing the generalized physical state is a complex-valued function of real variables.

Axiom III' (motion of (generalized) proper physical state) The law of motion of a proper physical system or a generalized proper physical system is determined by the Schrödinger equation.

We call the Schrödinger equation to be the equation of motion of this proper physical system or this generalized proper physical system. The Schrödinger equation is represented in the form

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

Here the operator H is of the same form as the Schrödinger operator for the total physical system.

Either in the case where H has only the discrete spectrum or in the case where H has a continuous spectrum, the Schrödinger equation has the same form formally in both cases.

When the Schrödinger operator has only the discrete spectrum, the L^2 -density, which determines the physical state of a total physical system, is determined by the eigenfunction expansion by using L^2 -densities which determine the proper physical states.

When the Schrödinger operator has a continuous spectrum, such a L^2 -density $\psi(\boldsymbol{r},t)$ is also determined by the generalized eigenfunction expansion by using L^2_{loc} -densities which determine the generalized proper physical states.

Thus, eventhough we use L^2 -densities or L^2_{loc} -densities as the physical states of the physical subsystems, the physical state of the total physical system is determined by the L^2 -density.

5 Derivation of Schrödinger Equations

5.1 Derivation of Schrödinger Equations (1)

At first, we consider the case where the Schrödinger operator H has only the discrete spectrum.

We define the energy expectation value of this physical system by the relation

$$J[\psi] = \int \left(\sum_{i=1}^n rac{\hbar^2}{2m_i} |\psi_{x_i}(oldsymbol{r})|^2 + V(oldsymbol{r}) |\psi(oldsymbol{r})|^2
ight) doldsymbol{r}.$$

In order that we determine the physical state which is realized physically in the real among all admissible physical state, we solve one problem of variation by virtue of the variational principle and derive the following Schrödinger equation as an Euler equation:

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

Now, by the inverse process of the method of seperation of variables, we have the Schrödinger equation depending on time t:

$$i\hbar\frac{\partial\psi}{\partial t} = \left\{-\sum_{i=1}^{n} \frac{\hbar^{2}}{2m_{i}} \frac{\partial^{2}}{\partial x_{i}^{2}} + V\right\}\psi.$$

5.2 Derivation of Schrödinger Equations (2)

Next, we consider the case where the Schrödinger operator H has a continuous spectrum.

For any compact set S in \mathbb{R}^n , we define the local energy expectation value of this physical system by the relation

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

In order that we determine the physical state which is realized physically in the real among all admissible $L^2_{\rm loc}$ -densities, we solve one problem of variation by virtue of the

local variational principle and derive the following Schrödinger equation as an Euler equation :

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

Now, by the inverse process of the method of seperation of variables, we have the Schrödinger equation depending on time t:

$$i\hbarrac{\partial\psi(m{r},t)}{\partial t}=\left\{-\sum_{i=1}^{n_i}rac{\hbar^2}{2m_i}rac{\partial^2}{\partial x_i^2}+V(m{r})
ight\}\psi(m{r},t).$$

6 Harmonic Oscillator

What is a harmonic oscillator?

A harmonic oscillator is not a microparticle as a natural existence such as an electron, an atom or an molecule.

It is, in fact, a mathematical model which represents a state of motion under which a microparticle as a natural existence is moving in a neighborhood of a stable eqilibilium point of the potential.

It is an approximating model for a motion of a real microparticle.

In fact, in a neighborhood of an stable eqilibilium point x = a, the potential V(x) can be approximated by a potential of the type of harmonic oscillator:

$$V(x) \doteqdot \frac{1}{2}V''(a)(x-a)^2.$$

In the one dimensional case, the Schrödinger equation in the stationary states for the considered physical system can be approximated by the Schrödinger equation

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + \frac{m}{2}\omega^2x^2\psi(x) = \mathcal{E}\psi(x).$$

In this case, the solutions are given in the following.

Theorem 6.1 There exists a complete orthonormal systems of eigenfunctions $\psi_n(x)$ and eigenvalues \mathcal{E}_n as follows:

$$\psi_n(x) = \sqrt{\frac{1}{2^n n!}} \sqrt{\frac{m\omega}{\pi\hbar}} \exp\left[-\frac{m\omega}{2\pi}x^2\right] H_n\left(\sqrt{\frac{m\omega}{\hbar}}x\right),$$

$$\mathcal{E}_n = \left(n + \frac{1}{2}\right)\hbar\omega,$$

$$(-\infty < x < \infty; n = 0, 1, 2, \cdots).$$

Here $H_n(\xi)$ is the Hermite polynomial

$$H_n(\xi) = (-1)^n e^{\xi^2} \frac{d^n}{d\xi^n} e^{-\xi^2}, \ (n = 0, 1, 2, \cdots).$$

We have the Schrödinger equation of time evolution of the system of harmonic oscillators as follows.

Theorem 6.2 There exists a unique solution $\psi(x,t)$ of the initial value problem of the Schrödinger equation of time evolution:

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

 $\psi(x,0) = \psi(x)$, (initial value condition),
 $(-\infty < x < \infty, \ 0 < t < \infty).$

Here $\psi(x)$ is a given L^2 -density.

7 Black Body Radiation and Planck's Formula of Radiation

Planck obtained his formula of radiation.

In the old quantum theory, this formula is derived using the model of the hollow-space radiation which is considered to be equivalent to the model of black body radiation.

But even if we can obtain the Planck's formula of radiation using the model of hollow-space radiation, it is not the proof of the fact that the black body itself is glowing by the cause of heat and is radiating the light.

We show here the true meaning of the black body radiation and the Planck's formula of radiation.

We show that we can derive Planck's formula of radiation by calculating the energy expectation value of the system of harmonic oscillators by using the L^2 -density. This L^2 -density is the solution of the Schrödinger equation of the system of harmonic oscillators.

Here we use the fact that we can consider the black body as the system of harmonic osillators approximately.

After all, we have the energy expectation value \overline{E}_M per 1 mol:

$$\overline{E}_{M} = rac{1}{2}N\hbar\omega + rac{N\hbar\omega}{\exp\left[rac{\hbar\omega}{k_{B}T}
ight] - 1}.$$

Here N is the Avogadro number and k_B is the Boltzman constant and T is the absolute temperature.

This is, in fact, the Planck's formula of radiation.

Then we prove the Wien's displacement law by using the hypothesis of light quantum.

Finally we found the problem: What is the light quantum?

This is the future problem.

8 Specific Heat of Solid Matter

Here we obtain a new explanation of the Debye's model of specific heat of a solid. We consider the molar heat of a monatomic solid spreaded infinitely in the 3-dimensional space.

Every atom of the solid is oscillating by the cause of heat.

Approximately we may consider every atom as a harmonic oscillator near the equilibrium point.

We consider that the solid is the system of harmonic oscillators with angular momentum ω , $(0 < \omega < \omega_D)$.

Here ω_D denotes the Debye frequency.

Then we obtain the energy expectation value of this physical system as follows:

$$\overline{E} = \frac{3}{2}N\hbar\overline{\omega} + 3N\int_0^\infty \frac{\hbar\omega}{\exp\left[\frac{\hbar\omega}{k_BT}\right] - 1}D(\omega)d\omega.$$

Here we put

$$\overline{\omega} = \int_0^\infty \omega D(\omega) d\omega,$$

where $D(\omega)$ denotes the probability density of ω .

Then we have the molar heat C as follows:

$$C = \frac{d\overline{E}}{dT} = 9Nk_B \left(\frac{T}{\theta_D}\right)^3 \int_0^{\theta_D/T} \frac{x^4 e^x}{(e^x - 1)^2} dx.$$

Here we put

$$heta_D = rac{\hbar \omega_D}{k_B}.$$

We call θ_D to be the Debye temperature.

The Debye model shows the good coincidence between the theoretical result and the experimental result. The Debye model gives a very good model of the true physical phenomena.

This gives the new meaning of the specific heat for the Debye model of a solid.

9 System of Free Particles

A free particle is a particle moving freely under no action of force. Thus the Newtonian equation of motion of a free particle with mass m is

$$m\frac{d^2x}{dt^2}=0.$$

We consider the system of free particles.

In this case, we have the Schrödinger equation

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} = \mathcal{E}\psi(x),$$
$$(-\infty < x < \infty).$$

Here we have the solutions in the following.

Theorem 9.1 There exists a complete orthonormal system of generalized eigenfunctions $\psi^{(p)}(x)$ and generalized eigenvalues \mathcal{E}_p as follows:

$$\psi^{(p)}(x) = \frac{1}{\sqrt{2\pi\hbar}}e^{ipx/\hbar}, \ \mathcal{E} = \frac{p^2}{2m},$$

$$(-\infty < x < \infty, -\infty < p < \infty).$$

We have the Schrödinger equation of time evolution of the system of free particles as follows.

Theorem 9.2 There exists a unique solution $\psi(x,t)$ of the initial value problem of the Schrödinger equation of time evolution:

$$i\hbar rac{\partial \psi(x,t)}{\partial t} = -rac{\hbar^2}{2m} rac{\partial^2 \psi(x,t)}{\partial x^2},$$
 $\psi(x,0) = \psi(x), ext{ (initial value condition)},$ $(-\infty < x < \infty, \ 0 < t < \infty).$

Here $\psi(x)$ is a given L^2 -density.

In the real, all natural existence is moving under the interaction of forces.

Therefore, the system of free particles is the idealized physical system.

But, in fact, the system of free particles is used to research the physical phenomena of the system of ideal gas as approximating model.

In this sense, the system of free particles which is considered only the mathematical model for a simple calculation corresponds to the concrete physical phenomena.

This fact is a very new result and very interesting.

10 Specific Heat of Ideal Gas

In this section, we consider the molar heat C_M and the specific heat C_V of constant volume of an ideal gas composed of monatomic molecules in the point of natural statistical physics.

We consider an ideal gas composed of monatomic molecules spreaded infinitely.

There N_V molecules in the region of volume V. The ideal gas is so rarefied that there is no mutual interaction among molecules. They only move freely and no forces act on them.

Every molecule moves under the Newtonian equation of motion:

$$m\frac{d^2x}{dt^2}=0.$$

Here m denotes the mass of one molecule.

So that, we consider this ideal gas to be the system of free particles.

Thus we have the Schrödinger equation:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} = \mathcal{E}\psi(x), \ (-\infty < x < \infty).$$

Then we have the Schrödinger equation of time evolution:

$$i\hbar rac{\partial \psi(x,t)}{\partial t} = -rac{\hbar^2}{2m} rac{\partial^2 \psi(x,t)}{\partial x^2},$$
 $\psi(x,0) = \psi(x), ext{ (initial value condition)},$ $(-\infty < x < \infty, \ 0 < t < \infty).$

By simple calculations, we have the energy expectation value of this system:

$$\overline{E}=\frac{3}{2}k_BT.$$

Thus we have the specific heat C_V of constant volume and the molar heat C_M of this ideal gas as follows:

$$C_V = N_V \frac{d\overline{E}}{dT}$$
 and $C_M = N \frac{d\overline{E}}{dT}$.

Here N denotes the Avogadro number.

Namely, we have

$$C_V = \frac{3}{2}N_V k_B$$
 and $C_M = \frac{3}{2}Nk_B$.

If we put $N_V = nN$, we have the relation

$$C_V = nC_M$$
.

11 Square Potential Barrier and Tunnel Effect

Here we consider the following physical system. Many electrons run through a long fine wire.

Each electron is considered to be a material point with electric charge.

Assume that we can disregard the mutual interaction between electrons.

Some force acts on these electrons. This force is given as the square potential barrier.

The potential V(x) is given as follows:

$$V(x) = \begin{cases} V, & (|x| \le a), \\ 0, & (|x| > a), \end{cases}$$

where a > 0 and V > 0.

Then electrons of low energy are rebounded by this force, and electrons of high energy go through the region of this potential by overcoming this force.

This phenomenum is called just a tunnel effect, and is understood as a natural statistical phenomenum.

This is considered as a principle of semiconductor diode.

Such a method of understanding the phenomenum of tunnel effect is clarified first by the natural statistical physics.

This is a very new understanding.

For this physical system, we have the Schrödinger equation

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + V(x)\psi(x) = \mathcal{E}\psi(x),$$

$$(\mathcal{E} \ge 0, \ -\infty < x < \infty).$$

We have the new solutions of this Schrödinger equation in the following Theorems 11.1 ~ 11.3 .

Theorem 11.1 Assume $V > \mathcal{E} \ge 0$, and put $\mathcal{E} = \frac{p^2}{2m}$, $(|p| < \sqrt{2mV})$. Then we have the solutions $\psi_1^{(p)}(x)$ and $\psi_2^{(p)}(x)$ as follows:

$$\psi_1^{(p)}(x) = \begin{cases} \frac{1}{\sqrt{\pi\hbar}} \sin(x-a)p/\hbar, & (x>a), \\ 0, & (|x| \le a), \\ -\frac{1}{\sqrt{\pi\hbar}} \sin(x+a)p/\hbar, & (x<-a), \end{cases}$$

$$\psi_2^{(p)}(x) = \begin{cases} \frac{1}{\sqrt{\pi\hbar}} \sin(x-a)p/\hbar, & (x>a), \\ 0, & (|x| \le a), \\ \frac{1}{\sqrt{\pi\hbar}} \sin(x+a)p/\hbar, & (x<-a). \end{cases}$$

Theorem 11.2 Assume $\mathcal{E} \geq V$, and put $\mathcal{E} = \frac{p^2}{2m} = \frac{p'^2}{2m} + V$, $(|p| \geq \sqrt{2mV}, -\infty < 1)$ $p'<\infty$).

Here we consider p' as a function of p.

Then we have the solution $\psi_1^{(p)}(x)$ as follows:

(i) When x > a, we have

$$\psi_1^{(p)}(x) = \frac{1}{\sqrt{\pi\hbar}} \left(\cos p' a/\hbar \cdot \cos p(x-a)/\hbar - \frac{p'}{p} \sin p' a/\hbar \cdot \sin p(x-a)/\hbar\right).$$

(ii) When x < -a, we have

$$\psi_1^{(p)}(x) = \frac{1}{\sqrt{\pi\hbar}} \left(\cos p' a/\hbar \cdot \cos p(x+a)/\hbar + \frac{p'}{p} \sin p' a/\hbar \cdot \sin p(x+a)/\hbar\right).$$

(iii) When $|x| \leq a$, we have

$$\psi_1^{(p)}(x) = \frac{1}{\sqrt{\pi\hbar}} \cos p' x/\hbar.$$

Theorem 11.3 Assume \mathcal{E} , p, p' be as same as in Theorem 11.2. Then we have the solution $\psi_2^{(p)}(x)$ as follows:

(iv) When x > a, we have

$$\psi_2^{(p)}(x) = \frac{1}{\sqrt{\pi\hbar}} \left(\sin p' a / \hbar \cdot \cos p(x-a) / \hbar + \frac{p'}{p} \cos p' a / \hbar \cdot \sin p(x-a) / \hbar \right).$$

(v) When x < -a, we have

$$\psi_2^{(p)}(x) = \frac{1}{\sqrt{\pi\hbar}} \left(\sin p' a / \hbar \cdot \cos p(x+a) / \hbar - \frac{p'}{p} \cos p' a / \hbar \cdot \sin p(x+a) / \hbar \right).$$

(vi) When $|x| \leq a$, we have

$$\psi_2^{(p)}(x) = \frac{1}{\sqrt{\pi\hbar}} \sin p' x/\hbar.$$

We have the following.

Theorem 11.4 There is a unique L^2 -density $\psi(x,t)$, depending on time t, of the initial value problem of the Schrödinger equation of time evolution:

$$i\hbar rac{\partial \psi(x,t)}{\partial t} = -rac{\hbar^2}{2m} rac{\partial^2 \psi(x,t)}{\partial x^2} + V(x)\psi(x,t),$$
 $\psi(x,0) = \psi(x)$, (initial value condition), $(-\infty < x < \infty, \ 0 < t < \infty).$

Here $\psi(x)$ is a given L^2 -density.

12 Potential Energy Well

Here we consider the following physical system. Many electrons run through a long fine wire.

Each electron is considered to be a material point with electric charge.

Assume that we can disregard the mutual interaction between electrons.

Some force acts on these electrons. This force is given as the potential energy well.

The potential V(x) is given approximately as follows:

$$V(x) = \begin{cases} -V, & (|x| \le a), \\ 0, & (|x| > a), \end{cases}$$

where a > 0 and V > 0.

Then each electron is moving by the Newtonian equation of motion:

$$m\frac{d^2x}{dt^2} = -\frac{dV(x)}{dx} = V\delta_{(-a)} - V\delta_{(a)}.$$

For this physical system, we have the Schrödinger equation

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + V(x)\psi(x) = \mathcal{E}\psi(x),$$
$$(-\infty < x < \infty).$$

We have the new solutions of this Schrödinger equation in the following Theorems 12.1 \sim 12.3.

Theorem 12.1 Assume $0 > \mathcal{E} \ge -V$, and put $\mathcal{E} = \frac{p^2}{2m} - V$, $(|p| < \sqrt{2mV})$. Then we have the solutions $\psi_1^{(p)}(x)$ and $\psi_2^{(p)}(x)$ as follows:

(i) When
$$p = \left(n + \frac{1}{2}\right) \frac{h}{2a}$$
, $(|p| < \sqrt{2mV}, n = 0, \pm 1, \pm 2, \cdots)$, we have

$$\psi_1^{(p)}(x) = \psi_1^{(n)}(x) = \begin{cases} \frac{1}{\sqrt{a}} \cos\left(n + \frac{1}{2}\right) \frac{\pi x}{a}, & (|x| \le a), \\ 0, & (|x| > a). \end{cases}$$

(ii) When $p = \frac{nh}{2a}$, $(|p| < \sqrt{2mV}, n = \pm 1, \pm 2, \cdots)$, we have

$$\psi_2^{(p)}(x) = \psi_2^{(n)}(x) = \begin{cases} \frac{1}{\sqrt{a}} \sin \frac{n\pi x}{a}, & (|x| \le a), \\ 0, & (|x| > a). \end{cases}$$

Theorem 12.2 Assume $\mathcal{E} \geq 0$, and put $\mathcal{E} = \frac{p^2}{2m} = \frac{p'^2}{2m} - V$, $(|p'| \geq \sqrt{2mV}, -\infty .$

Here p' is considered to be a function of p.

Then we have the solution $\psi_1^{(p)}(x)$ as follows:

(i) When x > a, we have

$$\psi_1^{(p)}(x) = \frac{1}{\sqrt{a}} \left(\cos p' a / \hbar \cdot \cos p(x-a) / \hbar - \frac{p'}{p} \sin p' a / \hbar \cdot \sin p(x-a) / \hbar \right).$$

(ii) When x < -a, we have

$$\psi_1^{(p)}(x) = \frac{1}{\sqrt{a}} \left(\cos p' a / \hbar \cdot \cos p(x+a) / \hbar + \frac{p'}{p} \sin p' a / \hbar \cdot \sin p(x+a) / \hbar \right).$$

(iii) When $|x| \leq a$, we have

$$\psi_1^{(p)}(x) = \frac{1}{\sqrt{a}} \cos p' x / \hbar.$$

Theorem 12.3 Assume \mathcal{E} , p, p' be as same as in Theorem 12.2. Then we have the solution $\psi_2^{(p)}(x)$ as follows:

(iv) When x > a, we have

$$\psi_2^{(p)}(x) = \frac{1}{\sqrt{a}} \left(\sin p' a / \hbar \cdot \cos p(x-a) / \hbar + \frac{p'}{p} \cos p' a / \hbar \cdot \sin p(x-a) / \hbar \right).$$

(v) When x < -a, we have

$$\psi_2^{(p)}(x) = \frac{1}{\sqrt{a}} \left(\sin p' a / \hbar \cdot \cos p(x+a) / \hbar \right. \\ \left. - \frac{p'}{p} \cos p' a / \hbar \cdot \sin p(x+a) / \hbar \right).$$

(vi) When $|x| \leq a$, we have

$$\psi_2^{(p)}(x) = \frac{1}{\sqrt{a}} \sin p' x / \hbar.$$

We have the following.

Theorem 12.4 There is a unique L^2 -density $\psi(x,t)$, depending on time t, of the initial value problem of the Schrödinger equation of time evolution:

$$i\hbar rac{\partial \psi(x,t)}{\partial t} = -rac{\hbar^2}{2m} rac{\partial^2 \psi(x,t)}{\partial x^2} + V(x)\psi(x,t),$$
 $\psi(x,0) = \psi(x)$, (initial value condition), $(-\infty < x < \infty, \ 0 < t < \infty).$

Here $\psi(x)$ is a given L^2 -density.

Potential Energy Well of Infinite Depth **13**

Here we consider the following physical system. Many electrons run through a fine wire of finite length.

Each electron is considered to be a material point with electric charge.

Assume that we can disregard the mutual interaction between electrons.

Assume that the both ends of the wire are the walls of complete reflection.

Some force acts on these electrons. This force is given as the potential energy well of infinite depth.

The potential V(x) is given approximately as follows:

$$V(x) = \begin{cases} 0, & (|x| \le a), \\ \infty, & (|x| > a), \end{cases}$$

where a > 0.

Then each electron is moving by the Newtonian equation of motion:

$$m\frac{d^2x}{dt^2} = 0, \ (|x| \le a).$$

Each electron is moving with constant velocity. So that this motion is considered to be periodic.

For this physical system, we have the Schrödinger equation with periodic condition:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} = \mathcal{E}\psi(x),$$

$$(\mathcal{E} > 0, |x| < a).$$

 $\psi(-a) = \psi(a)$, (boundary value condition).

We have the new solutions of this Schrödinger equation in the following.

Theorem 13.1 We have the new solutions $\psi_1^{(p)}(x)$ and $\psi_2^{(p)}(x)$, $(|x| \leq a)$ as follows:

(1)
$$\psi_1^{(0)}(x) = \frac{1}{\sqrt{2a}}$$
.
(2) $\psi_1^{(n)}(x) = \frac{1}{\sqrt{a}} \cos \frac{n\pi x}{a}$, $(n = 1, 2, \cdots)$.
(3) $\psi_2^{(n)}(x) = \frac{1}{\sqrt{a}} \sin \frac{n\pi x}{a}$, $(n = 1, 2, \cdots)$.

Here we put $p = \frac{n\pi\hbar}{a} = \frac{nh}{2a}$, $(n = 0, 1, 2, \cdots)$.

We have the following.

Theorem 13.2 There is a unique L^2 -density $\psi(x,t)$, depending on time t, of the initial and boundary value problem of the Schrödinger equation of time evolution:

$$i\hbar rac{\partial \psi(x,t)}{\partial t} = -rac{\hbar^2}{2m} rac{\partial^2 \psi(x,t)}{\partial x^2},$$

 $\psi(x,0) = \psi(x)$, (initial value condition),

$$(|x| \le a, \ 0 < t < \infty),$$

 $\psi(-a) = \psi(a), \ \psi(-a,t) = \psi(a,t), \ (0 < t < \infty), \ (boundary value condition).$

Here $\psi(x)$ is a given L^2 -density.

14 Experiment of Double Slits

Here we consider the experiment of double slits by using the theory of the natural statistical physics.

We consider the 1-dimensional mathematical model of this phenomena.

We consider the systems of electrons moving in \mathbb{R}^1 under the potential V(x).

Each electron is considered to be a material point with electric charge.

Assume that we can disregard the mutual interaction between electrons.

For this physical system, we have the Schrödinger equation of time evolution:

$$i\hbarrac{\partial\psi(x,t)}{\partial t}=-rac{\hbar^2}{2m}rac{\partial^2\psi(x,t)}{\partial x^2}+V(x)\psi(x,t),$$

$$\psi(x,0) = \psi(x)$$
, (initial value condition),
 $(-\infty < x < \infty, \ 0 < t < \infty)$.

Here we choose $\psi(x)$ as follows.

We consider two small intervals S_1 and S_2 in \mathbb{R}^1 , which is considered to be two slits. All electrons run through either one of two slits.

So that we have two physical subsystems:

one is the subsystem of electrons which run through the slit S_1 and the other is the subsystem of electrons which run through the slit S_2 .

The initial conditions of these two subsystems are given by $\psi_1(x)$ and $\psi_2(x)$ whose supports are in S_1 and S_2 , respectively.

Then we put

$$\psi(x) = \alpha \psi_1(x) + \beta \psi_2(x),$$
$$|\alpha|^2 + |\beta|^2 = 1, \ (-\infty < x < \infty, \ \alpha, \beta \in \mathbf{C}).$$

Then we have the L^2 -densities $\psi_1(x,t)$, $\psi_2(x,t)$ and $\psi(x,t)$ as the solutions of the Schrödinger equation of time evolution corresponding to the initial value conditions $\psi_1(x)$, $\psi_2(x)$ and $\psi(x)$ respectively.

Then we have the relation

$$\psi(x,t) = \alpha \psi_1(x,t) + \beta \psi_2(x,t).$$

Then the electrons are distributed on the screen following the probability density

$$|\psi(x,t)|^2 = |\alpha|^2 |\psi_1(x,t)|^2 + \alpha^* \beta \psi_1(x,t)^* \psi_2(x,t) + \beta^* \alpha \psi_2(x,t)^* \psi_1(x,t) + |\beta|^2 |\psi_2(x,t)|^2.$$

This is observed as the same pattern as that of intervention of waves.

By this result, we can understand the meaning of experiment of double slits.

Thereby we can understand the meaning of Tonomura's experiment.

15 Spectrum of Hydrogen Atoms

Here we consider the spectrum of the hydrogen atoms by using the theory of the natural statistical physics.

We consider the system of hydrogen atoms by excluding the influence of the spin.

There are the case where there is not the influence of the exterior electromagnetic field or the case where we can disregard such a influence.

Each hydrogen atom is the system of two particles, composed of one proton and one electron revolving around the proton.

Each electron is moving in the 3-dimensional space.

Assume that we can disregard the mutual interaction between different hydrogen atoms.

The mass of the proton is very bigger than the mass of the electron.

Therefore we can consider the system of the hydrogen atoms to be the system of free electrons moving under the Coulomb potential field $V(r) = -\frac{e^2}{r}$.

Then, for this system of hydrogen atoms, we have the Schrödinger equation descriving the statinary states of the systems of free electrons:

$$\left(-rac{\hbar^2}{2m}\Delta-rac{e^2}{r}
ight)\psi(m{r})=\mathcal{E}\psi(m{r}),$$

where $\Delta = \Delta r$ denotes the Laplace operator with respect to r and we put r = |r|. Further we denote the mass of an electron as m.

Then we have the following.

Theorem 15.1 We have the solutions $\psi_{nlm}(r)$ of the Schrödinger equation :

$$\left(-\frac{\hbar^2}{2m} \Delta - \frac{e^2}{r} \right) \psi_{nlm}(r) = \mathcal{E}_n \psi_{nlm}(r),$$

$$(|m| \le l, \ l = 0, 1, \cdots, n - 1; \ n = 1, 2, \cdots),$$

$$\mathcal{E}_n = -\frac{me^4}{2\hbar^2 n^2}, \ (n = 1, 2, \cdots),$$

$$\psi_{nlm}(r) = \psi_{nlm}(r, \theta, \phi) = R_{nl}(r) Y_l^m(\theta, \phi),$$

$$R_{nl}(r) = -\left\{ \left(\frac{2}{na_0} \right)^3 \frac{(n - l - 1)!}{2n[(n + l)!]^3} \right\}^{1/2} e^{-s/2} s^l L_{n+l}^{(2l+1)}(s),$$

$$Y_l^m(\theta, \phi) = \sqrt{\frac{(2l+1)}{4\pi} \frac{(l - |m|)!}{(l+|m|)!}} P_l^m(\cos \theta) e^{im\phi}.$$

Here we put

$$a_0 = \frac{\hbar^2}{me^4}, \ s = \frac{2}{na_0}r.$$

In the above, the function $L_n^{(m)}(z)$ is a Laguerre bipolynomial defined by the relation

$$L_n^{(m)}(z) = \frac{1}{n!} z^{-m} e^z \frac{d^n}{dz^n} (z^{n+m} e^{-z}),$$

 $(n = 0, 1, 2, \dots m = 1, 2, \dots).$

For the Schrödinger equation of the system of hydrogen atoms under the bound state, we have the following.

Theorem 15.2 We have a unique solution $\psi(r,t)$ of the initial value problem of the Schrödinger equation of time evolution:

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

 $\psi(\boldsymbol{r},0) = \psi(\boldsymbol{r}), \text{ (initial value condition)},$
 $(\boldsymbol{r} \in \boldsymbol{R}^3).$

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

After all, each hydrogen atom composing the physical subsystem of mean energy \mathcal{E}_n varies its belonging to the physical subsystems with the passage of time.

Thus, when some hydrogen atom belonging to the subsystem of mean energy \mathcal{E}_n moves to the subsystem of mean energy \mathcal{E}_m , we observe the spectral line corresponding to the difference of mean energies

$$\mathcal{E}_n - \mathcal{E}_m$$
.

This coincides with the distribution of the observed spectrum of the hydrogen atoms in the real.

This fact coincides with the historically known fact by virtue of Bohr's hypothesis.

We have known many sequences of spectra of hydrogen atoms such as Lyman, Balmer, Ritz-Paschen, Brackett and Pfund.

16 Philosophy of Natural Statistical Physics

We cannot give the detail of this philosophy in this small space. So that, in this time, we only refer to my book, Y. Ito[5], Chapter 14.

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