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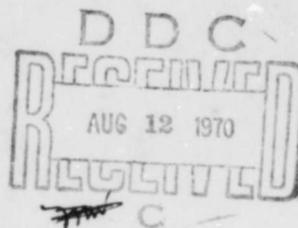
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DIFFICULTY AND POSSIBILITY OF
KINETIC THEORY OF QUANTUM-MECHANICAL SYSTEMS

Part II — The Quantum-mechanical
Liouville Equation and Its Solutions

by

Toyoki Koga



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and
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SUMMARY

The theme of this report is a problem of correlation, as is illustrated in section I by considering the two-electron problem according to the Schrodinger equation. In section II, the Schrodinger equation is reduced to a partial differential equation which is equivalent to the classical Liouville equation, to the approximation of nullifying \hbar^2 in the former. An energy eigen-function of the Schrodinger equation corresponds to the representation of a microcanonical ensemble of classical-mechanical systems in the phase space. For example, the energy eigen function of the electron in a one-electron atom corresponds to a microcanonical ensemble of single-particle systems in the classical-mechanical sense. The uncertainty existing in the quantum-mechanical representation of a particle is two-fold: A part of the uncertainty stems from our intention to describe the behavior of the particle, which is likely to have an extension in the six-dimensional phase-space, in

*The comment of Dr. Arthur E. Ruark given on this matter has been most stimulating.

terms of the concept of classical material point; it also stems from the situation that we are treating an ensemble when we assume that we are treating a single particle. If this were not the case, we would have no way to explain strange kinetic-theoretical phenomena, which really exist and fail to arise from the application of conventional theories. In view of the above, the kinetic theory of quantum-mechanical systems is difficult to rely on standard solutions of the Schrodinger equation. Rather, at the present time, it seems most reasonable to utilize quasi-classical models of particles. The present discussion provides some legitimacy and significance to those models. Finally, the present interpretation of quantum mechanical phenomena provokes no disturbance in the conventional structure of the quantum-mechanical interpretation of the Schrodinger equation, so far as the conventional application of solutions of the equation is concerned.

I. INTRODUCTION

In Part I of this report, it is discussed that there is a possibility of kinetic theory of quantum-mechanical systems, since there are evidences that the validity of the Pauli principle is localized. Nevertheless, we soon realize that it is not so easy to consider kinetic theory of quantum-mechanical systems. The situation is explained in the following.

Suppose that we have a two-electron system, as the simplest case. We may write down the Schrodinger equation for the system. This two-body problem is quite different from the

classical two-body problem. In the present case, we cannot define the relative velocity, the center of mass, etc. of the two electrons, and hence there is no way to simplify the problem by changing the coordinate system. (If one of the two particles were a heavy atom, there would be a way of justification of doing so, as we really do for calculating the electron energy of an atom.) The Hartree-Fock method has nothing to do about the difficulty, since we do not want to introduce the additional statistical sense all at once. Finally, we suppose that, to the zeroth approximation, the wave function of each electron is a plane wave: $\psi_0^1(r_1), \psi_0^2(r_2)$. Then we construct a wave function for the whole system,

$$\psi_0 = \psi_0^1(r_1)\psi_0^2(r_2) - \psi_0^1(r_2)\psi_0^2(r_1)$$

To the next approximation, we write $\psi_1 = \psi_0 + \varphi$, and substitute ψ_0 for ψ in the interaction term of the Schrodinger equation, and simply φ in the other terms. It is not yet a simple equation, but we suppose that we get a solution for φ . Is this the correct solution for the present problem? It is easily seen that this solution implies that the two electrons are interacting mutually at any time and anywhere in the same way; each electron appears to have been ground to a sort of powder of extremely small grain and spread uniformly in the entire space. Is this the real mode of the interaction between two electrons? The situation does not change as depending on the amount of energy contained in the system. In other words, we cannot switch this to the classical two-body problem, as long as we use those wave functions.

We remember that we meet a similar situation in the classical kinetic theory, if we use an ensemble representation of a system. (Ref.1). But we cannot simply conclude that the

situation of quantum-mechanical kinetic theory is analogous to the classical case. In this report, we investigate the matter more closely, by utilizing the quantum-mechanical Liouville equation which is derived from the Schrodinger equation, and attempt to find a feasible way of kinetic theory of quantum-mechanical systems.

II. DEDUCTION OF THE LIOUVILLE EQUATION FROM THE SCHRODINGER EQUATION

It has been known that the Wigner equation which is derived from the Schrodinger equation by a method of Fourier transformation is equivalent to the classical Liouville equation to the approximation that the term involving \hbar is ignored and the potential is expandable in a Taylor series, and its first derivative is retained. Ref.2. However, the procedure of the derivation is not analogous to the classical one, and hence it is difficult to see the physical correspondence between the two. In this section we also derive a partial differential equation from the Schrodinger equation. This equation is equivalent to the classical Liouville equation to the approximation of nullifying \hbar^2 , not \hbar , in the former. Besides, the procedure of derivation of this quantum-mechanical Liouville equation is much analogous to the derivation of the classical Liouville equation according to the Hamilton formalism. Hence we can see rather easily the correspondence, physical and mathematical, between the two equations, classical and quantal. In the following, the introductory part, down

to Eq.(2.3)', is well known. See Ref. 3.

We write the Schrodinger equation for a particle in a potential field U as follows:

$$i\hbar \frac{\partial \psi}{\partial t} = - \frac{\hbar^2}{2m} \Delta \psi + U \psi \quad (2.1)$$

$$\hbar = h/2\pi$$

We substitute in the above

$$\psi = a \exp(iS/\hbar) \quad (2.2)$$

where a and S are real functions of t and \vec{r} ; $\vec{r} = x, y, z$. (Any function which can be expressed as a sum of real and imaginary parts may be written as (2.2).) On considering the real part and the imaginary part in the equation separately, we have

$$\partial S/\partial t + (\text{grad } S)^2/2m + U - \hbar^2 \Delta a/(2ma) = 0 \quad (2.3)$$

$$\partial a^2/\partial t + \text{div}(a^2 \text{grad } S/m) = 0 \quad (2.4)$$

To the approximation of ignoring \hbar^2 , Eq.(2.3) yields

$$\partial S/\partial t + (\text{grad } S)^2/2m + U = 0 \quad (2.3)'$$

In the following, it will be shown that first Eqs.(2.3)' and (2.4) lead to the classical Liouville equation and second Eqs.(2.3) and (2.4) lead to a partial differential equation which may be called the quantum-mechanical Liouville equation.

1. The classical Liouville equation.

Equation (2.3)' is the Hamilton-Jacobi equation. The H-J equation implies Newton dynamics under certain additional conditions. Without the conditions, the H-J equation is a differential equation of broader implication. We first derive the Liouville equation in the classical sense, by introducing the additional conditions.

We suppose that we obtain a "complete" integral of Eq.(2.3)', a solution containing three arbitrary constants in addition to an additive constant:

$$S(\vec{r}, t, \alpha_1, \alpha_2, \alpha_3) + S_0$$

See Ref.4. From now on, we shall ignore constant S_0 . Then we define \vec{p} and $\beta_1, \beta_2, \beta_3$ by

$$\vec{p} = \text{grad } S \quad (2.5)$$

$$\beta_1 = -\frac{\partial S}{\partial \alpha_1}, \quad \beta_2 = -\frac{\partial S}{\partial \alpha_2}, \quad \beta_3 = -\frac{\partial S}{\partial \alpha_3} \quad (2.6)$$

In order to let \vec{p} imply momentum, it is necessary to put that

$$\frac{d\alpha_\nu}{dt} = 0, \quad \frac{d\beta_\nu}{dt} = 0, \quad \nu = 1, 2, 3 \quad (2.7)$$

(These conditions are not contained in the H-J equation.) According to (2.5), the components of \vec{p} are functions of \vec{r} , t and the α 's:

$$\begin{aligned} p_x &= p_x(\vec{r}, t, \alpha) \\ p_y &= p_y(\vec{r}, t, \alpha) \\ p_z &= p_z(\vec{r}, t, \alpha) \end{aligned} \quad (2.8)$$

Similarly, the β 's are

$$\begin{aligned} \beta_1 &= \beta_1(\vec{r}, t, \alpha) \\ \beta_2 &= \beta_2(\vec{r}, t, \alpha) \\ \beta_3 &= \beta_3(\vec{r}, t, \alpha) \end{aligned} \quad (2.9)$$

By eliminating x, y, z from those six equations, we may obtain the p 's as functions of the α 's and β 's and t :

$$\begin{aligned}
P_x &= p_x(\alpha, \beta, t) \\
P_y &= p_y(\alpha, \beta, t) \\
P_z &= p_z(\alpha, \beta, t)
\end{aligned}
\tag{2.10}$$

and subsequently, Eqs.(2.8) yield

$$\begin{aligned}
x &= x(\alpha, \beta, t) \\
y &= y(\alpha, \beta, t) \\
z &= z(\alpha, \beta, t)
\end{aligned}
\tag{2.11}$$

These six functions give the trajectory of a particle in accordance with the Newton dynamics. Since there are six constants, the α 's and β 's, involved in those functions of t , one may choose the p 's at time t as independent of the choice of x, y, z . If we define H by

$$H = (\text{grad } S)^2 / (2m) + U = \vec{p}^2 / 2m + U$$

then, according to (2.3)' and (2.5), we have

$$(\vec{dp}/dt)_r = - \text{grad } H = - \text{grad } U \tag{2.12}$$

where $(\)_r$ means that the derivative is made under the condition that r is fixed.* (If we wish to do so, we may take the α 's for the three initial coordinates and the β 's for the three initial components of momentum.)

We consider Eq.(2.4) in terms of the solution of Eq.(2.3)' considered in the above. Considering (2.5) and that \vec{p} and \vec{r} are mutually independent, in accordance with (2.10) and (2.11), we write for Eq.(2.4)

$$(\partial a^2 / \partial t)_r + (\vec{p}/m) \cdot \text{grad } a^2 = 0 \tag{2.4}'$$

In this presentation, \vec{p} is a function of the α 's, β 's and t . By solving this equation, we suppose, we obtain a "complete"

*This is the initial definition of d/dt in Eq.(2.3).

solution which contains three more additional constants

$\delta_1, \delta_2, \delta_3$:

$$a^2 = \rho(\vec{r}, t, \alpha, \beta, \delta) \quad (2.13)$$

where α means the α 's. By means of (2.10), however, we may eliminate either the α 's or the β 's and bring in the p 's instead. Suppose we eliminate the α 's. Then we obtain a function of $\vec{r}, \vec{p}, t, \beta, \delta$ for a^2 :

$$a^2 = \rho(\vec{r}, \vec{p}, t, \beta, \delta) \quad (2.14)$$

If we rewrite Eq.(2.4)' in terms of this function, we have to write

$$\frac{\partial}{\partial t} + (dp/dt)_r \cdot \frac{\partial}{\partial \vec{p}}$$

in the place of $\partial/\partial t$. Then, on consideration of (2.12), we may write for Eq.(2.4)'

$$\left(\frac{\partial}{\partial t} + \frac{\vec{p}}{m} \cdot \text{grad} - \text{grad } U \cdot \frac{\partial}{\partial \vec{p}} \right) \rho = 0 \quad (2.15)$$

This is the Liouville equation in the classical-mechanical sense.

2. The Liouville equation in the quantum-mechanical sense.

From Eqs.(2.3) and (2.4), we may derive the Liouville equation in the quantum-mechanical sense, as analogous to the classical one. Since Eq.(2.3) contains a , we have to solve the two equations simultaneously. Suppose that we have a set of "complete" solutions which contain six arbitrary constants:

$$S(\vec{r}, t, \alpha, \delta), \quad a(\vec{r}, t, \alpha, \delta)$$

where

$$\vec{r} = x, y, z, \quad \alpha = \alpha_1, \alpha_2, \alpha_3, \quad \delta = \delta_1, \delta_2, \delta_3$$

Then we define \vec{p} and the β 's by

$$\vec{p} = \text{grad } S \quad (2.16)$$

$$\beta_1 = -\partial S / \partial \alpha_1, \quad \beta_2 = -\partial S / \partial \alpha_2, \quad \beta_3 = -\partial S / \partial \alpha_3 \quad (2.17)$$

Here \vec{p} is simply a vector variable and does not necessarily mean momentum. According to (2.16), we have

$$\begin{aligned} p_x &= p_x(\vec{r}, t, \alpha, \gamma) \\ p_y &= p_y(\vec{r}, t, \alpha, \gamma) \\ p_z &= p_z(\vec{r}, t, \alpha, \gamma) \end{aligned} \quad (2.18)$$

and according to (2.17)

$$\begin{aligned} \beta_1 &= \beta_1(\vec{r}, t, \alpha, \gamma) \\ \beta_2 &= \beta_2(\vec{r}, t, \alpha, \gamma) \\ \beta_3 &= \beta_3(\vec{r}, t, \alpha, \gamma) \end{aligned} \quad (2.19)$$

We regard the β 's as invariant, in the same way as in the classical case. By eliminating \vec{r} from (2.18) and (2.19), we obtain

$$\begin{aligned} p_x &= p_x(\alpha, \beta, \gamma, t) \\ p_y &= p_y(\alpha, \beta, \gamma, t) \\ p_z &= p_z(\alpha, \beta, \gamma, t) \end{aligned} \quad (2.20)$$

and then, substituting the above in Eq.(2.18), we obtain

$$\begin{aligned} x &= x(\alpha, \beta, \gamma, t) \\ y &= y(\alpha, \beta, \gamma, t) \\ z &= z(\alpha, \beta, \gamma, t) \end{aligned} \quad (2.21)$$

\vec{p} and \vec{r} are independent, since they contain nine constants. (See the statement following Eq.(2.11).) Further, by solving (2.20) with respect to the α 's and substituting the result in $a(\vec{r}, t, \alpha, \gamma)$, we obtain

$$a = a(\vec{r}, \vec{p}, t, \beta, \gamma) \quad (2.22)$$

If we substitute the above for a in Eq.(2.4), operator $\partial/\partial t$ has to be read

$$\partial/\partial t + (d\vec{p}/dt)_{\vec{r}} \cdot \partial/\partial \vec{p}$$

Hence, Eq.(2.4) yields

$$\frac{\partial a^2}{\partial t} + \left(\frac{d\vec{p}}{dt} \right)_{\vec{r}} \cdot \frac{\partial a^2}{\partial \vec{p}} + \frac{\vec{p}}{m} \cdot \frac{\partial a^2}{\partial \vec{r}} = 0 \quad (2.23)$$

We may calculate $(d\vec{p}/dt)_{\vec{r}}$ from Eq.(2.3) where t and \vec{r} are mutually independent. First, operate operator grad:

$$\partial (\text{grad } S)/\partial t + \text{grad} (\text{grad } S)^2/2m + \text{grad } U - \frac{\hbar^2}{2m} \text{grad}(\Delta a/a) = 0$$

Considering $\vec{p} = \text{grad } S$, we obtain

$$(d\vec{p}/dt)_{\vec{r}} + \text{grad } U - \frac{\hbar^2}{2m} \text{grad}(\Delta a/a) = 0 \quad (2.24)$$

On eliminating $(d\vec{p}/dt)_{\vec{r}}$ from (2.23) and (2.24), we have

$$\frac{\partial a^2}{\partial t} - (\text{grad } U - \frac{\hbar^2}{2m} \text{grad}(\Delta a/a)) \cdot \frac{\partial a^2}{\partial \vec{p}} + \frac{\vec{p}}{m} \cdot \frac{\partial a^2}{\partial \vec{r}} = 0 \quad (2.25)$$

This may be regarded as the Liouville equation in the quantum-mechanical sense.

It is noted that the Wigner equation, derived also from the Schrodinger equation, is equivalent to the classical Liouville equation to the approximation of nullifying \hbar , not \hbar^2 , if the potential U is expandable in a Taylor series of distance and its first derivative is retained. See Ref.2. The difference between the Wigner equation and Eq.(2.25) may be attributed to the difference between the definitions of \vec{p} . The present equation is more advantageous in the sense that its connection to the classical one is explicit and natural.

We may perform the same reduction as in the above, with respect to the Schrodinger equation for a many-particle system.

III. SOLUTIONS OF THE CLASSICAL LIOUVILLE EQUATION

In the classical Liouville equation (2.15), variables t, \vec{r}, \vec{p} are independent. ($\vec{r} = x, y, z, \vec{p} = p_x, p_y, p_z$.) Therefore, in general, a solution of the equation is a function of those independent variables. As we change arbitrarily the values of those variables, ρ changes accordingly. If we impose a certain relation between those changes of independent variables, however, ρ may not change. The relation is given by the characteristic equations of Eq.(2.15):

$$\begin{aligned} dt &= \frac{dx}{p_x/m} = \frac{dy}{p_y/m} = \frac{dz}{p_z/m} \\ &= - \frac{dp_x}{\partial U/\partial x} = - \frac{dp_y}{\partial U/\partial y} = - \frac{dp_z}{\partial U/\partial z} \end{aligned} \quad (3.1)$$

In other words, if the changes occur according to (3.1), ρ does not change. Equation (3.1) are the Newton equations of dynamics. We note the following: Suppose that we have a solution of Eq.(2.15), a function of \vec{r}, \vec{p} and t . By equalizing the solution to a constant, say A , we obtain an equation

$$\rho(\vec{r}, \vec{p}, t) = A$$

This equation should be satisfied by a set of solutions of (3.1). But we cannot derive (3.1) from this equation.

In the following, we shall discuss three typical solutions of Eq.(2.15):

1. Solution for a single system.

$$\begin{aligned} \rho_1 &= \int_0^\infty \delta(x - x(t)) \delta(y - y(t)) \delta(z - z(t)) \times \\ &\quad \times \delta(p_x - p_x(t)) \delta(p_y - p_y(t)) \delta(p_z - p_z(t)) \\ &\quad (\rho_1 = \text{const}) \end{aligned} \quad (3.2)$$

This function, δ function, satisfies the Liouville equation (2.15), if $x(t)$, $y(t)$, $z(t)$, $p_x(t)$, $p_y(t)$, $p_z(t)$ are solutions of Eqs.(3.1), and x, y, z, p_x, p_y, p_z are independent variables. Function (3.2) represents a single system in the phase space.

2. Ensembles in general.

From (3.2), we may generate a solution which represents a group of similar systems (ensemble). In (3.2), those functions of time t

$$x(t), y(t), z(t), p_x(t), p_y(t), p_z(t)$$

contain their initial values denoted by

$$x_0, y_0, z_0, p_{x0}, p_{y0}, p_{z0}$$

If the initial density distribution of the group of the systems is given by

$$\varphi(x_0, y_0, z_0, p_{x0}, p_{y0}, p_{z0}) \quad (3.3)$$

then

$$\rho = \iiint \iiint \iiint \varphi \rho_i dx_0 dy_0 dz_0 dp_{x0} dp_{y0} dp_{z0} \quad (3.4)$$

is the solution which we wish to obtain.

3. Micro-canonical ensemble.

If we take for ρ

$$\rho = a^2 = f(U + p^2/2m) \quad (3.5)$$

we see easily that this satisfies Eq.(2.15). In order to make this as the representation of a microcanonical ensemble, an additional condition is necessary, that is

$$U + p^2/2m = E = \text{const} \quad (3.6)$$

This is equivalent to taking for S in Eq.(2.3)'

$$S = -Et + s \quad (3.7)$$

where E is constant and s is independent of t . By (3.7), equation (2.3)' yields

$$-E + p^2/2m + U = 0 \quad (3.6)$$

In summary, the following are significant: a) The characteristic equations are independent of ρ . b) A characteristic line does not cross another line.

We may consider the same with respect to many-particle systems.

IV. SOLUTIONS OF THE SCHRÖDINGER EQUATIONS AND THE CORRESPONDING SOLUTIONS OF THE CLASSICAL LIOUVILLE EQUATION.*

The Liouville eq.(2.15) is linear and of the first order. But equation (2.25) which may be called the quantal Liouville equation is neither linear nor of the first order.

We begin our investigation by assuming that $(h^2/2m)\text{grad}(\frac{\Delta a}{a})$ in the equation is a minor correction term. Then we may think that the classical equation (2.15) is the substitute of Eq.(2.25) to the first approximation. Then, on substitution of the first approximate solution of a in the correction term, we may consider Eq.(2.25) as linear and of the first order. After repeating successively similar processes of approximation, we may define a trajectory by

*Those speculations, made in this section and unnecessary in the standard quantum mechanics, are merely for the convenience for the discussion in section V.

$$\frac{d\vec{p}}{dt} = -\text{grad } U + \frac{\hbar^2}{2m} \text{grad} \left(\frac{\Delta a}{a} \right)$$

$$\frac{d\vec{r}}{dt} = \frac{\vec{p}}{m} \quad (4.1)$$

These are characteristic equations of Eq.(2.25) to the present approximation. It is rather obvious that we cannot call a line, determined in the phase space according to (4.1), as "trajectory" of a particle, because here the trajectory appears to be affected by a or by other systems and the situation is contradictory to the definition of ensemble that a system belonging to an ensemble should not be affected by another system belonging to the same ensemble. The only feasible interpretation is that the behavior of a system (a particle in this case) is represented by a bundle of these characteristic lines, instead of a single line*. At a moment of time, a finite domain of the 6-dimensional phase space represents a state of a particle. According to the present interpretation, a^2 may be the representation of an ensemble of systems which do not interfere mutually, only when each finite domain of the relevant phase space representing a state of a system is separated from the others in function a^2 at each moment of time. One representative domain of the phase space should be occupied only by one system at a moment of time. (The situation is similar to the situation of many billiard balls which are on the same table and do not collide mutually.) If this condition is not satisfied, a trajectory may violently deviate from any of the physically possible ones because of the interference which should not occur on a system in the ensemble, and the situation causes singularity of a^2 .

Thus far, we have been assuming that we solve Eq.(2.25) by a method of successive approximation, simply for the

*A similar interpretation was proposed earlier by de Broglie. See Ref. 3. The term containing a in (4.1) should belong to the concerned particle itself.

purpose of understanding the effect of the non-linear terms in Eq.(2.25). The method of successive approximation is not practical, however: We do not know, in advance of solution, how should the first approximation be set, such that the convergency of the final result is assured. If we obtain an exact solution all at once and the solution does not contain any singularity, we may expect that the solution be physically significant.

1. Energy Eigen-solutions.

An energy eigen-function of the Schrodinger equation is given by

$$\psi(x,y,z,t) = a \exp(iS/\hbar) \quad (4.2)$$

where $S = -Et + s$ (4.3)

and E is constant, s and a are independent of t . Then we have

$$i\hbar \partial\psi/\partial t = E\psi$$

On this understanding, we substitute (4.2) in Eqs.(2.3) and (2.4), obtaining

$$-E + U + (\text{grad } s)^2/2m - \hbar^2 \Delta a/(2ma) = 0 \quad (4.4)$$

$$\partial a^2/\partial t = 0, \quad \text{div}(a^2 \text{grad } s/m) = 0 \quad (4.5)$$

According to the definition of \vec{p} made in section II, we may rewrite (4.4) and (4.5), and obtain*

$$-E + U + p^2/2m - \hbar^2 \Delta a/(2ma) = 0 \quad (4.4)'$$

$$\left. \begin{aligned} \partial a^2/\partial t - [\text{grad } U - (\hbar^2/2m) \text{grad}(\Delta a/a)] \cdot \partial a^2/\partial \vec{p} &= 0 \\ \vec{p} \cdot \text{grad } a^2 &= 0 \end{aligned} \right\} \quad (4.5)'$$

Due to the introduction of p , a may be a function of t .

If we nullify \hbar^2 in the above, Eq.(4.4)' implies the energy conservation in the classical sense, and this condition determines a surface in the phase space. On the surface, a^2 may change in such a way that Eqs.(4.5)' are satisfied. This is the representation of a microcanonical ensemble. As far as those conditions are satisfied, we may choose the distribution of a^2 arbitrarily.

If a is independent of \vec{r} , we have

$$i\hbar \partial\psi/\partial \vec{r} = (\text{grad } s)\psi = \vec{p}\psi$$

In this case, $\hbar^2 \Delta a/(2ma)$ in (4.4)' disappears.

The situation is shown by Eq.(3.5), where we may choose function f and E as we wish. a^2 (or f) represents a superposition of various trajectories possible under condition (3.6).

If the term containing h in Eq.(4.4)' is significant, the distribution of a also affects the energy law of the system under consideration (a particle in this case). According to the interpretation made in the beginning of this section, a feasible solution is expected to exist only under a restrictive condition. Indeed, according to Schrodinger, the possible values of E , in the case of an electron in an atom for example, are strictly specified, and only for each of such values of E , a^2 and S are possible to be determined uniquely, with no singularity. An eigen function thus determined in the configuration space gives us only a vague information of the behavior of the system under consideration. The vagueness stems from two causes: 1) The state of a particle at a moment of time is represented by a^2 and S in a finite domain of the phase space, and consequently a trajectory of the particle, not only in the configuration space but also in the phase space, is not a line but a bundle of lines. 2) Many possible trajectories, each representing a possible and entire history (cycle) of the system, are superposed in one configuration space, as well as in the relevant phase space, and represent a microcanonical ensemble*. (The first cause is found only in a quantum-mechanical system. But the second cause exists also with respect to a classical system.) Thus a^2 appears to represent a cloud spread in the entire configuration space. The present interpretation is obviously different from Born's interpretation**. Born attributed the peculiar characteristic of the cloud, which is partly (or mainly?) the characteristic of an ensemble even in the classical sense,

*In the Schrodinger solution, the magnitude and direction of angular momentum are also specified.. But the direction of apogee is not specified.

**The reader may complain the author, because our interpretation produces nothing new so far as the standard problems of quantum mechanics are concerned. But in section V, we shall see the significance.

to the assumed peculiarity of quantum-mechanical particles.

See Ref. 5. (In his classical kinetic theory, Born is not sensitive of ensemble. Ref. 1.)

2. Wave packet and plane wave.

It is often said that a wave packet which satisfies the Schrodinger equation represents a free particle.

If $U = 0$ in the Schrodinger equation (2.1), we have for a solution

$$\exp (i p_x x / \hbar - i E t / \hbar) \quad (4.6)$$

$$E = p_x^2 / 2m \quad (4.7)$$

Consequently, the Fourier transform of G , a function of p_x / mc

$$\psi (xt) = \int_{-\infty}^{+\infty} G(p_x / mc) \exp (i \frac{p_x x}{\hbar} - i \frac{E t}{\hbar}) d(p_x / mc) \quad (4.8)$$

is also a solution. If we choose G properly, ψ represents a localized wave (one-dimensional wave packet), although unstable*. See Ref. 6. At the limit $\hbar \rightarrow 0$, the wave packet appears to be a plane, placed perpendicularly to the x -axis and moving in the x -direction. We may construct a three-dimensional wave packet which may represent a particle.

If we distribute many similar wave packets in the three-dimensional configuration space, and the distribution is made with a certain regularity as depending on function G , we obtain a plane wave to an approximation:

$$\psi = a \exp (i p_{x0} x / \hbar - i E_0 t / \hbar) \quad (4.9)$$

* Should this instability be attributed to the nature of a particle or to the imperfection of the Schrodinger equation? Some arbitrariness permissible in the choice of G suggests the latter.

where p_{x0}/m is the group velocity of a packet, and $E_0 = p_{x0}^2/2m$. Since amplitude a in (4.9) is substantially constant, the corresponding classical ensemble consists of similar one-particle systems distributed uniformly in the 3-dimensional configuration space. At this classical limit, we cannot detect the regularity or order given primarily to the distribution of the wave packets, as necessary for forming the plane wave (4.9). In an ensemble, each system (a particle in this case) should not interact with any other system (a particle), no matter how closely they may be located in the space. This demand of the definition of ensemble and the conventional mathematical scheme of representation are compatible, so far as classical material points are concerned. But it is not so with respect to quantal particles, as is manifest in Eq.(4.1). The regularity imposed on the distribution of wave packets is a mathematical convenience, but is an unnecessary restriction from the view-point of physics. For example, if we suppose that a beam of electrons is represented by an ensemble of single-particle systems, the only necessary condition is that each electron in the beam is independent of the others. We cannot expect that the distribution of those electrons in the beam should be regulated in the same way as the distribution of those wave packets is for making a plane wave. In other words, a plane wave is simply a representation of a single particle for a certain purpose specified in quantum-mechanics.

As Dr. Ruark once pointed out to the author, those speculations made in this section are all unnecessary (meaningless) for solving the conventional problems of quantum-mechanics. Nothing, new and significant, may be developed from them. They may be rather disgusting in the sense that that miraculous beauty and perfection of the system of quantum mechanics be unnecessarily destroyed by them. Nevertheless, the author thinks that those speculations are necessary for solving kinetic-theoretical problems such as demonstrated in the next section.

V. FROM THE KINETIC-THEORETICAL VIEW POINT

Thus far, we have seen that there are good mathematical correspondences between quantum-mechanical solutions of the Schrodinger equation and ensemble solutions of the classical Liouville equation. Thus far, however, we have not said that those solutions of the Schrodinger equation represent ensembles. For it is merely nominal and insignificant to do so from the physical view point, so far as those conventional solutions are concerned. In the following, however, we shall show that the same physical significance as seen of the difference between ensemble and single system in classical mechanics is also found of the difference between mathematically nominated ensemble and mathematically nominated single system in quantum mechanics, treating a kinetic phenomenon.

We suppose that we have two similar electron beams in a large vacuum chamber. Each of them is well collimated. One beam is set along the x-axis and the other along the y-axis of our imaginary coordinate system. We may call them respectively the X beam and the Y beam. They intersect mutually in the domain surrounding the origin of the coordinate axes. We wish to investigate the mode of the interaction by means of the Schrodinger equation. Quantum mechanics suggest the following two methods:

Method I.

We represent each of the two beams with a plane wave, to the zeroth approximation: The X beam with ψ_x^0 and the Y beam by ψ_y^0 . It is obvious that $\psi_x^0 \psi_y^0$ satisfies the relevant Schrodinger equation where the interaction term is neglected. (There are only two independent coordinate variables x, y in the equation.) To the next approximation, we substitute $\psi_x^0 \psi_y^0$ in the interaction term and $\psi_x^0 \psi_y^0 + \psi$ in the other terms

of the Schrodinger equation. Thus we have a partial differential equation where ψ is unknown. φ gives the effect of the interaction between the two beams. Although we do not solve the equation for ψ in this report, it is not difficult to guess the essential characteristic of the result. The beams are both retarded as they approach toward the intersection and are accelerated after leaving the intersection. The effect of crossing is expected only in a space near the intersection. (Also we have to consider the interaction between one part of a beam and another part of the same beam. This effect has no direct relation to the purpose of the present discussion. Note, the beams are well collimated.) The interaction is very smooth; there is no abrupt interaction.

Method II.

We assume, to the zeroth approximation, that each electron is represented by a wave packet. (Since the velocity of each beam is large and our observation is limited to the vicinity of the intersection, each packet may be assumed to be stable.) Each beam consists of many similar wave packets, in the same way as a gas consists of classical molecules. The wave function of the whole system is the product of all the wave-packet representations:

$$\psi^0 = \prod \psi_n^0 \quad n=1,2,3,\dots$$

ψ^0 satisfies the Schrodinger equation where the interaction terms are neglected. It should be noted that, unlike the case of Method I, the independent variables are t , and x_1, x_2, x_3, \dots for the X beam and y_1, y_2, y_3, \dots for the Y beam. Each wave packet contains t and one spatial coordinate. Therefore, the Schrodinger equation contains many interaction terms for all the pairs of those coordinates. To the next approximation, we do the same as we did in Method I. ψ^0 is substituted in the interaction

terms, and $\psi^0 + \varphi$ in the other terms of the Schrodinger equation. Here again, we do not solve the equation. But we can predict the result according to our experience of classical gas theory. In this case, the energy, momentum and charge of each electron are not spread over the entire beam, but instead are concentrated within a tiny wave packet. Hence there is a possibility that an electron in the X beam and an electron in the Y beam interact violently and abruptly, like two particles colliding according to the classical dynamics. As a result, an electron after interaction may not stay in the beam where it belongs; instead it may run out to a completely different direction. The detail is fairly well known by the classical kinetic theory, and is omitted here.

After studying comparatively the two methods, we realize that, the physical characteristic of problem I is quite similar to the characteristic of the problem of treating a classical-mechanical system in terms of its ensemble representation. On the other hand, the situation in problem II is similar to the situation of a classical mechanical system when treated as a single system. (In classical kinetic theory, ensemble representation is not useful. See Ref. 1.)

We may now believe that the correspondence found in section IV does not remain merely as mathematical, but the correspondence manifests itself in physical phenomena. Our conclusion is that those speculations made in section IV have physical significance, when we investigate kinetic-theoretical phenomena which have been being ignored by the conventional quantum mechanics.

The reader might ask, what is the feasible approach of kinetic theory? The possible and most reasonable way, at this time, of kinetic theory seems to rely on quasi-classical models of particles. There is a reason for being optimistic about this approach: A system which we are interested in from the kinetic-theoretical view-point tends to contain a comparative-

ly large amount of energy, and quasi-classical models may well simulate real particles constituting the system.

VI. CONCLUDING REMARK

In this report, our interpretation of quantum-mechanical phenomena has gone somehow beyond the standard one, and possibly might have provoked some uneasiness in the reader. However, we should note that the present discussion has done nothing to antagonize the authorized or standard interpretation of quantum mechanics, so far as the conventional problems are concerned. As is simply stressed in section V, if we wish to investigate a group of phenomena, which may be called kinetic-theoretical, we have to make up an interpretation which is compatible with the standard one and yet possible to give feasible solutions for those strange problems. This is what we have discussed in this report. If the reader could take the matter in this sense, the author would be most grateful.

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APPENDIX
 A COMPLETE SET OF ORTHOGONAL EIGEN FUNCTIONS
 IN THE CONFIGURATION SPACE AND IN THE PHASE SPACE

In the following, \vec{p} does not mean momentum in the classical sense, but instead is simply a variable defined by (2.16). Hence, the discussion is merely mathematical, so far as this section is concerned. However, it has physical meanings when coope rating with section V.

According to Eqs.(4.2) and (4.3), we write those eigen functions as follows:

$$\psi_k = a_k \exp(-iE_k t/\hbar) \exp(is_k/\hbar) \quad (\text{A.1})$$

$$k = 1, 2, 3, \dots$$

Here, E_1, E_2, \dots are respectively constants, and $a_1, s_1, a_2, s_2, \dots$ are functions of $\vec{r} = x, y, z$ while being independent of t . However, if we introduce $\vec{p}_1, \vec{p}_2, \dots$ as defined by (2.16), a_k, s_k appear to be dependent of time t , as is shown by (4.5)'. This is due to a transformation among invariants as is stated with respect to (2.22):

$$\begin{aligned} a_k(\vec{r}, \alpha_k, \delta_k) &= a_k(\vec{r}, \vec{p}, t, \beta_k, \gamma_k) \\ s_k(\vec{r}, \alpha_k, \delta_k) &= s_k(\vec{r}, \vec{p}, t, \beta_k, \gamma_k) \end{aligned} \quad (\text{A.2})$$

$$k = 1, 2, \dots$$

In the rp -space, function $a_k(r, \alpha_k, \delta_k)$ is an envelope of function $a_k(r, p, t, \beta_k, \gamma_k)$ as is illustrated schematically in Fig.1.

Since the E 's are constants, the orthogonal relations among the ψ 's are given by

$$\int a_k a_{k'} \exp [i(s_k - s_{k'})/\hbar] dr = 0 \quad (\text{A.3})$$

$$k \neq k'$$

In the configuration space (r -space), each function $a_k(r, \alpha_k, \delta_k)$ covers the entire space. But in the pr -space, they are separable.

As we know well, the domains are completely separable in the classical case. But, because of a involved in Eq.(4.4)', they may be partly overlapped in this case. Nevertheless, at each moment of time, they are distinguishable if p is defined by

$$\vec{p}(r, t, \beta_k, \delta_k) \quad (A.4)$$

according to (2.20) and (2.21), where (β_k, δ_k) is different from one eigenfunction to another. The situation is schematically illustrated in Fig.2.



Fig.1. The solid line represents $a_k(r, \alpha_k, \delta_k) = \text{const.}$ Each dotted line represents $a_k(r, p, t, \beta_k, \delta_k) = \text{const.}$ at each different time, t', t'', \dots

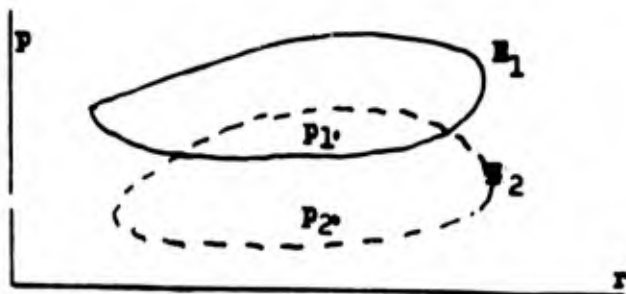


Fig.2. The domain of eigenfunction of E_1 is represented by the domain enclosed by solid line, and the domain of eigenfunction of E_2 by the domain by dotted line. Since a is involved in Eq.(4.4)', they may be overlapped, in general. But, if r and t are given, the values of p , (A.4), are different in two cases of E .

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Abstract (Continued)

interpretation of quantum mechanical phenomena provokes no disturbance in the conventional structure of the quantum-mechanical interpretation of the Schrodinger equation, so far as the conventional application of the solutions of the equation are concerned.