

THE HYDRODYNAMICAL MODEL OF WAVE MECHANICS I

THE MOTION OF A SINGLE PARTICLE IN A POTENTIAL FIELD

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The problem is investigated as to how far the wave equation representing a quantum-mechanical system can be transformed by change of variables into a system of equations which have the form of the classical equation of motion of a deformable medium. In the present paper we carry out this investigation in the case of a single charged particle moving under the influence of an outside potential.

I. Basic conceptions

§ 1. The difficulties connected with the physical interpretation of the wave function ψ have renewed interest in the hydrodynamical model of wave mechanics, i.e. in a model in which the fundamental equations of motion refer to classical quantities by which ψ may be replaced. Summarizing our considerations to be presented in a number of papers, we shall analyse the problem of how far it is possible to replace the wave mechanical description of a system by one mathematically equivalent and of the form of the classical equations of motion of an elastic medium.

Our attempt is not new, similar considerations have been given already e.g. by MADELUNG [1] and later by EHRENFEST [2] and TAKABAYASI [3]. (See also our short communication [4].) Further a number of papers have been published in connection with the classical analogy of quantum mechanics which are to a certain degree similar to ours as regards the mathematical formalism but which are different as regards their aim. (We mention here e.g. L. DE BROGLIE [5] and K. NOVOBÁTZKY [6].) On another occasion we shall summarize the wide literature on the subject.

§ 2. The simplest case, i.e. the motion of a particle of mass m and charge e under the influence of forces which can be derived from a potential V can be described by the SCHRÖDINGER wave equation

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

where the wave function ψ is a function of the coordinates and of the time. We may write for short $\psi(\mathbf{r}, t) = \psi$. Similarly V may depend on both \mathbf{r} and t , thus we may write $V(\mathbf{r}, t) = V$.

According to the generally accepted interpretation of the wave function $|\psi|^2$ is a probability density, i.e. $|\psi|^2 d\tau$ is the probability to find the particle (which is supposed to be pointlike) inside the volume element $d\tau$ [7]. SCHRÖDINGER's original idea [8] was that $|\psi|^2$ represents a true density, i.e. the particle is smeared over space with a mass density ϱ_m and electric charge density ϱ_e so that

$$\varrho_m = m\varrho, \quad \varrho_e = e\varrho \quad \text{with} \quad \varrho = |\psi|^2. \quad (2)$$

Later, reluctantly, SCHRÖDINGER had to give up his original idea and to accept BORN's probability interpretation.

The considerations connected with the hydrodynamical model automatically renew the question as to the interpretation of $|\psi|^2$. The density defined by (2) appears as one of the variables of the hydrodynamical model, thus the classical picture of the system described by the wave function corresponds to a medium with density $\varrho = \varrho(\mathbf{r}, t)$ spread out over space and moving under the influence of outer forces, the elastic stresses occurring inside the medium.

§ 3. SCHRÖDINGER already pointed out that the velocity of flow can be expressed in terms of ψ as follows:

$$\varrho\mathbf{v} = -\frac{i\hbar}{2m}(\psi^* \text{grad} \psi - \psi \text{grad} \psi^*). \quad (3)$$

The quantities defined by (2) and (3) satisfy together with (1) the following relation

$$\text{div}(\varrho\mathbf{v}) + \frac{\partial\varrho}{\partial t} = 0. \quad (4)$$

This is the so-called continuity equation, which can be derived from the SCHRÖDINGER equation. Thus \mathbf{v} and ϱ can be taken to describe velocity and density distribution of a moving medium.

It should be noted that adding a term $\text{rot} \chi$ (where χ is some arbitrary vector quantity) to the definition (3) of \mathbf{v} , the continuity equation (4) would also be satisfied. In the present approximation we may take this term to be zero. We shall return to the exact determination of the form of χ when dealing with the hydrodynamical model describing the electron having spin and magnetic moment, i.e. when χ can be determined by comparison with the experimental results.

Multiplying (4) by m and e , respectively, we obtain the continuity equation for the flow of mass $\text{div} \mathbf{p} + \frac{\partial\varrho_m}{\partial t} = 0$ and that for the electric

current $\operatorname{div} \mathbf{i} + \frac{\partial \varrho_e}{\partial t} = 0$, we merely have to suppose

$$\begin{aligned} \mathbf{p} &= m\varrho\mathbf{v} = \varrho_m\mathbf{v}, \\ \mathbf{i} &= e\varrho\mathbf{v} = \varrho_e\mathbf{v}, \end{aligned} \quad (5)$$

where \mathbf{p} is the density of momentum and \mathbf{i} the density of electric current in suitable units.

Integrating (4) over the whole of space (changing in the second term the order of integration and differentiation and supposing that $\varrho\mathbf{v}$ tends sufficiently strongly to zero at infinity), we find

$$\frac{d}{dt} \int \varrho d\tau = 0.$$

Thus the density integrated over the whole space is constant in time and — to be compatible with the wave equation — has to be given the value 1, i.e.

$$\int \varrho d\tau = 1. \quad (6)$$

Using the normalization (6) we obtain for total mass and total charge of the medium the initially given values m and e .

II. Equation of motion

§ 4. So as to obtain a dynamical description of our system it is necessary to consider the acceleration of the elements of the medium. According to hydrodynamics the acceleration of an element of a moving medium is given by the total derivative of the velocity, i.e.

$$\mathbf{a} = \frac{d\mathbf{v}}{dt} = \frac{\partial\mathbf{v}}{\partial t} + (\mathbf{v} \operatorname{grad}) \mathbf{v}, \quad (7)$$

where the partial derivative $\frac{\partial\mathbf{v}}{\partial t}$ expresses the rate of change of velocity in a fixed point. Instead of (7) we can also write, taking into account the continuity equation (4):

$$\varrho \frac{d\mathbf{v}}{dt} = \frac{\partial(\varrho\mathbf{v})}{\partial t} + \operatorname{Div}(\varrho\mathbf{v} \circ \mathbf{v}), \quad (8)$$

where Div is the tensor divergence and \circ designates the direct product.

Differentiating (3) with respect to time and expressing the time derivatives of ψ^* and ψ in terms of their spatial derivatives with help of the wave equ. (1), we get from (8):

$$\varrho_m \frac{d\mathbf{v}}{dt} = -\varrho \operatorname{grad} (V + Q) \quad (9)$$

with

$$Q = -\frac{\hbar^2}{2m} \frac{\nabla^2 \varrho^{1/2}}{\varrho^{1/2}}. \quad (10)$$

In place of (9) and (10) one may also write

$$\varrho_m \frac{d\mathbf{v}}{dt} = -\varrho \operatorname{grad} V - \operatorname{Div} \mathfrak{D}, \quad (9a)$$

with the tensor given by the relation

$$\mathfrak{D} = -\frac{\hbar^2}{4m} \varrho (\nabla \circ \nabla) \ln \varrho \quad (10a)$$

or writing down the i, k -th component of the tensor

$$Q_{ik} = -\frac{\hbar^2}{4m} \varrho \frac{\partial^2 \ln \varrho}{\partial x_i \partial x_k}.$$

We find that equs. (9), (10) [or (9a) and (10a)] together with the continuity equation (4) give a complete set of equations of motion. Indeed, if we impose an initial condition upon \mathbf{v} and ϱ

$$\mathbf{v}(\mathbf{r}, 0) = \mathbf{v}_0(\mathbf{r}) \quad \text{and} \quad \varrho(\mathbf{r}, 0) = \varrho_0(\mathbf{r})$$

their time distribution can be determined uniquely from the above system of equations.

§ 5. The equs. (4), (9) and (10) are exactly of the form which is to be expected for the classical equations of motion of an elastic medium. Q plays the role of an inner potential and

$$\mathbf{F}_i = -\operatorname{grad} Q \quad (11)$$

is the stress appearing as the result of deformation.

That \mathbf{F}_i as given by (11) can be regarded as classical stress can be seen from the following remarks:

1. If $\varrho = \text{const.}$, then $Q = \text{const.}$ and $F_i = 0$, thus stress appears only at places where the density of the medium is non-uniform. In a given point, Q depends only upon the density in this point and the spatial derivatives of the density, thus we may say that Q in a given point is determined by the density distribution in the immediate vicinity of that point, just as is to be expected in an elastic medium.

2. It follows from (11) and (10) [or (10a)] that

$$\int \varrho \mathbf{F}_i d\tau = 0, \quad (12)$$

i.e. the inner forces resulting from the stress have no resultant. Thus the rate of change of momentum of the system is given by the integral over the outer forces only; or denoting by

$$\mathbf{R} = \int \varrho \mathbf{r} d\tau$$

the coordinate vector of the centre of gravity of our system, we find

$$m\ddot{\mathbf{R}} = \dot{\mathbf{P}} = \int \varrho \mathbf{F}_o d\tau, \quad (13)$$

where

$$\mathbf{F}_o = -\text{grad } V. \quad (13a)$$

Equation (13) expresses the law of EHRENFEST.

3. The moment of force produced by the inner forces can be written

$$\mathbf{K}_i = \int \varrho [\mathbf{r} \times \mathbf{F}_i] d\tau = - \int [\mathbf{r} \times \text{Div } \mathfrak{D}] d\tau.$$

Integrating by parts, we find, remembering that \mathfrak{D} is a symmetric tensor [see (10a)]:

$$\mathbf{K}_i = 0.$$

Thus the inner forces produce no moment of force. We find therefore for the total moment of force of the system in analogy to (13):

$$\mathbf{K} = \int \varrho [\mathbf{r} \times \mathbf{F}_o] d\tau, \quad (14)$$

i.e. the change of angular momentum is caused by the moment of the outer forces only. In particular, we note that the angular momentum of the system will change continuously provided the outer forces produce a non-vanishing moment.

Taking together the three remarks made above, we see that the equs (4), (9) and (10) describing the motion of our medium are indeed of the type of classical equations of motion. The fact that the constant \hbar appears in the expression giving the potential Q does not affect the classical nature of the equation. Indeed, \hbar may be regarded as a constant characteristic of the elastic properties of an atomic system. Obviously no description can be successful which does not make use of \hbar .

III. Connection between hydrodynamical equations and the wave equation

§ 6. In the following we discuss how far it is possible to establish a one to one correspondence between the descriptions of a system by a wave function on the one hand and the hydrodynamical variables ϱ and \mathbf{v} on the other.

For this purpose it is convenient to express the wave function ψ with help of two real functions $R = R(r, t)$ and $S = S(r, t)$ in the form

$$\psi = Re^{iS}. \quad (15)$$

Introducing (15) into the expressions for the density (2) we find

$$\varrho = R^2 \quad (16a)$$

and further from equ. (3) for the velocity of flow

$$\mathbf{v} = \frac{\hbar}{m} \text{grad } S. \quad (16b)$$

(It should be noted that the above expression for \mathbf{v} is valid only for points in which $\varrho \neq 0$; at points where $\varrho = 0$, \mathbf{v} may have singularities.)

If, however, we want to determine from given distributions of ϱ and \mathbf{v} the wave function ψ satisfying the wave equation, we have to express R and S through ϱ and \mathbf{v} . Reversing (16) we obtain

$$R = \sqrt{\varrho}, \quad (17a)$$

$$S = \frac{m}{\hbar} \int_{\mathbf{r}_0}^{\mathbf{r}} \mathbf{v} \, d\mathbf{r} + S_0, \quad (17b)$$

where \mathbf{r}_0 is a constant vector and S_0 a function of time only. Thus from a given distribution of ϱ and \mathbf{v} functions R and S may be determined on the

basis of (17), and further using (15) the corresponding ψ function fulfilling the wave equation may be built up. If we require ψ to be a single-valued function of the coordinates according to (15) \mathbf{v} may still be multi-valued having values differing by integer multiples of 2π from each other, i.e.

$$\oint \mathbf{v} d\mathbf{r} = 2\pi\hbar \frac{k}{m}, \quad k = 0, \pm 1, \pm 2, \dots, \quad (18)$$

where the path of integration must avoid points for which $\varrho = 0$, otherwise it may be an arbitrary closed path. The expression (18) relating to the velocity, together with the normalization (6) of the density may be regarded as initial conditions. Indeed (as can be shown easily), if they are fulfilled at a time $t = 0$ they remain so for all later times.

Equ. (18) is equal to Thomson's law of vortices in a field.

§ 7. So as to check whether ψ constructed from the distributions of ϱ and \mathbf{v} obeys indeed the wave equation, we insert the ψ function thus obtained into the wave equation. Doing so we find that the wave equation is indeed fulfilled, provided we take \mathbf{r}_0 to be an arbitrary vector independent of time and put

$$S_0 = -\frac{1}{\hbar} \int_0^t E(t) dt$$

with

$$E = \left(V + Q + \frac{1}{2} m\mathbf{v}^2 \right)_{\mathbf{r}=\mathbf{r}_0}.$$

Thus the explicit expression for ψ satisfying (1) can be written

$$\psi = \sqrt{\varrho} \exp \left\{ \frac{i}{\hbar} \int_{\mathbf{r}_0}^{\mathbf{r}} \mathbf{v} d\mathbf{r} - \frac{i}{\hbar} \int_0^t E(t) dt \right\}.$$

We see thus that owing to the arbitrary value of \mathbf{r}_0 , ψ is determined except for a constant phase factor; thus ψ may be replaced by $\psi' = \psi e^{i\gamma}$ (with $\nabla\gamma = \dot{\gamma} = 0$), ψ' corresponding to the same hydrodynamical distribution as ψ . However, in the usual considerations of wave mechanics such a phase factor is regarded as unimportant, thus we can conclude that essentially there exists a one to one correspondence between the solutions of the wave equation and the hydrodynamical equations (4), (9) provided only solutions obeying initial conditions (6), (18) are considered.

IV. Stationary states

§ 8. The Schrödinger wave equation (1) admits so-called stationary solutions of the form

$$\psi(\mathbf{r}, t) = \varphi(\mathbf{r}) e^{-\frac{i}{\hbar} E t} \quad (19)$$

when the potential energy $V(\mathbf{r})$ does not depend on the time.

The amplitude of the n -th stationary solution is determined by the equation

$$-\frac{\hbar^2}{2m} \nabla^2 \varphi_n + V \varphi_n = E_n \varphi_n, \quad (20)$$

where the constants E_n are the energy eigenvalues and the functions φ_n are the normalized eigenfunctions.

The corresponding hydrodynamical variables are of course independent of time, i.e. introducing (19) into (2) and (3) we get for the density and velocity of flow, respectively:

$$\begin{aligned} \varrho &= \varphi_n^*(\mathbf{r}) \varphi_n(\mathbf{r}), \\ \varrho \mathbf{v} &= -\frac{i\hbar}{2m} [\varphi_n^*(\mathbf{r}) \nabla \varphi_n(\mathbf{r}) - \nabla \varphi_n^*(\mathbf{r}) \varphi_n(\mathbf{r})]. \end{aligned} \quad (21)$$

a) Let us consider first the case when the amplitude of the stationary solution is real, i.e. $\varphi_n(\mathbf{r}) = \varphi_n^*(\mathbf{r})$. (It should be noted that a function ψ of real amplitude multiplied by a constant phase factor can also be regarded as a real solution in accordance with what we have said above.) As can be seen from (21) in this case

$$\frac{\partial \varrho}{\partial t} = 0 \quad \text{and} \quad \mathbf{v} = 0,$$

which means that the real stationary solutions correspond to states in which the medium representing the particle considered is at rest. The inner potential can be expressed with help of the amplitude function, taking into account (2), (10) and (19) in the form

$$Q = -\frac{\hbar^2}{2m} \frac{\nabla^2 \varphi_n(\mathbf{r})}{\varphi_n(\mathbf{r})}.$$

Using the amplitude equation (20) we have

$$Q = E_n - V$$

or forming the gradient and taking into account (11), (13)

$$\mathbf{F}_o + \mathbf{F}_i = 0,$$

i.e. the stress produced by the inner forces exactly balances the outer forces arising from the potential V .

A well-known example for this case is provided by the ground state of the H-atom. The inner potential corresponding to the wave function $\varphi_1(r) = Ce^{-\frac{r}{r_H}}$ has the form

$$Q = -\frac{me^4}{2\hbar^2} + \frac{e^2}{r} = E_1 - V(r),$$

where E_1 is the energy constant of the ground state and $V(r)$ represents the Coulomb potential. As can be seen Q obtained for this case produces a stress which exactly compensates the Coulomb attraction of the nucleus. The medium is in a state of stress but does not move.

b) Essentially complex solutions of the amplitude equation (20) correspond to states, where

$$\frac{\partial \varrho}{\partial t} = 0, \quad \mathbf{v} = -\frac{i\hbar}{2m} \text{grad} \ln \frac{\varphi_n(r)}{\varphi_n^*(r)}.$$

In such a state $\mathbf{v} \neq 0$, but $\frac{\partial \mathbf{v}}{\partial t} = 0$, these are characteristic expressions for a stationary flow.

As both the charge density ϱ_e and the current density i are constant in time, such a configuration produces stationary electric and magnetic fields, it does, however, not radiate.

For such a distribution $\text{grad}(V + Q) \neq 0$, i.e. the inner stress does not compensate exactly the outer force. We find with help of (7) and (9):

$$m(\mathbf{v} \text{grad}) \mathbf{v} = -\text{grad}(V + Q).$$

As can be seen easily, the uncompensated stress produces forces which are necessary to maintain the state of stationary flow.

A simple example for this case is provided by the $2p^1$ state of the H-atom to which belongs the wave function

$$\varphi_2(r) = C \frac{x + iy}{2r_H} e^{-\frac{r}{2r_H}}.$$

We find in this case

$$V + Q = E_2 - \frac{\hbar^2}{2m} \frac{1}{x^2 + y^2}$$

(with the energy constant of the $2p^1$ state: $E_2 = -\frac{me^4}{8\hbar^2}$). Thus as can be seen easily from this equation the inner and outer forces do not compensate each other and there remains an uncompensated attractive force, which varies proportional to $(x^2 + y^2)^{-3/2}$.

We find further, introducing $\varphi_2(r)$ into (3), that the medium rotates around the z -axis. The angular velocity in a point \mathbf{r} is given by

$$\omega = \frac{\hbar}{m} \frac{1}{x^2 + y^2}.$$

The centripetal force, which is needed to make the elements move along circular paths with such velocities is provided by that part of the stress which is not compensated by the Coulomb attraction of the nucleus and which has the form

$$F_C = m \omega^2 (x^2 + y^2)^{1/2} = \frac{\hbar^2}{m} (x^2 + y^2)^{-3/2}.$$

§ 9. Solutions of the wave equation (1) can be represented as linear combinations of stationary solutions. Thus a solution $\psi(\mathbf{r}, t)$ can be written in the form:

$$\psi(\mathbf{r}, t) = \sum c_\nu \varphi_\nu(\mathbf{r}) e^{-\frac{i}{\hbar} E_\nu t}, \quad (22)$$

where the stationary solutions form a normalized set. The corresponding charge and current densities can be obtained when introducing (22) into (2) and (3); we get thus:

$$\varrho = \sum \varrho_{\nu\mu} \cos(\omega_{\nu\mu} t + \alpha_{\nu\mu}), \quad (23)$$

where

$$\omega_{\nu\mu} = \frac{E_\nu - E_\mu}{\hbar} \quad (24)$$

and $\varrho_{\nu\mu}$, $\alpha_{\nu\mu}$ are functions of the coordinates only, i.e.

$$\begin{aligned} \varrho_{\nu\mu} &= |c_\nu c_\mu \varphi_\nu(\mathbf{r}) \varphi_\mu(\mathbf{r})|, \\ \alpha_{\nu\mu} &= \frac{1}{2i} \ln \frac{c_\mu c_\nu^* \varphi_\mu \varphi_\nu^*}{c_\mu^* c_\nu \varphi_\mu^* \varphi_\nu}. \end{aligned}$$

Similarly we find

$$\mathbf{p} = \sum \mathbf{p}_{\nu\mu} \cos(\omega_{\nu\mu} t + \beta_{\nu\mu}), \quad (25)$$

where the $\mathbf{p}_{\nu\mu}$ and $\beta_{\nu\mu}$ can be also expressed explicitly in terms of the c_ν and φ_ν .

Eqs. (23), (24) and (25) show that the medium in the non-stationary state vibrates with frequencies $\omega_{\nu\mu}$, which are exactly the Bohr frequencies. The terms with $\nu = \mu$ represent a constant charge and current density. This stationary motion is superimposed by the oscillation.

We see thus that the fluid representing the particle under investigation has its equilibrium configurations given by the eigenfunctions of the stationary states.

On the effect of some outer disturbance the medium starts to oscillate with frequencies $\omega_{\nu\mu}$ around its equilibrium configuration and as the medium is charged it emits electromagnetic radiation of those frequencies. The total dipole moment which is responsible for the emitted radiation can be written in the form:

$$\mathbf{d}_{\nu\mu} = -2c_\nu c_\mu e \int \mathbf{r} q_\nu^* q_\mu d\tau.$$

Frequencies belonging to a vanishing dipole moment do not occur in first approximation. Indeed, the current distribution inside the atom in a state described by the wave function

$$\psi = c_1 \varphi_1 e^{-\frac{i}{\hbar} E_1 t} + c_2 \varphi_2 e^{-\frac{i}{\hbar} E_2 t}$$

in the case $\mathbf{d}_{12} = 0$ is such that part of the medium oscillates with frequency ω_{12} , the phases of the oscillation being distributed in such a way that the radiation emitted by one part of the charged medium is opposite in phase to that emitted by the remaining part and in a first approximation the radiations emitted by the two parts extinguish each other by interference.

Considering the second approximation we obtain the so-called quadrupole radiation. Such a quadrupole radiation with its characteristic distribution of intensity and polarization is indeed observed in case of the forbidden lines when $\mathbf{d}_{\nu\mu} = 0$.

We note that the hydrodynamical model accounts also for the "elastically bound electron" which was postulated by HERTZ to explain the optical properties of atoms.

The main difficulty encountered by HERTZ was to explain how it is possible that an electron could be excited so as to vibrate with a series of frequencies.

This difficulty is overcome by the hydrodynamical concept. It is seen that the elastic forces derived from the inner potential Q together with the outside potential V provide a dynamical system, the characteristic frequencies of which are exactly the optical frequencies. Further, the modes of vibration

of this system are in accordance with the polarization and intensity distribution of the observed spectral lines.

In a later article we shall present our considerations for the case when the electromagnetic field is also taken into account. Following on this we shall deal with the hydrodynamical model of the electron with spin.

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ГИДРОДИНАМИЧЕСКАЯ МОДЕЛЬ ВОЛНОВОЙ МЕХАНИКИ I

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Резюме

Рассматривается проблема о возможностях преобразования, путём замены переменных, волнового уравнения квантовомеханической системы в систему уравнений, обладающую формой классического уравнения движения деформирующейся среды. В представленной работе мы изучаем этот вопрос для одной заряженной частицы, движущейся под влиянием внешнего потенциала.