I.2 ON THE QUANTUM MECHANICS OF COLLISIONS

[Preliminary communication][†]

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> Through the investigation of collisions it is argued that quantum
> mechanics in the Schrödinger form allows one to describe not only
> stationary states but also quantum jumps.

Heisenberg's quantum mechanics has so far been applied exclusively to the calculation of stationary states and vibration amplitudes associated with transitions (I purposely avoid the word "transition probabilities"). In this connection the formalism, further developed in the meantime, seems to be well validated. However, questions of this kind deal with only one aspect of quantum theory. Beside them there shows up as equally important the question of the nature of the "transitions" themselves. On this point opinions seem to be divided. Many assume that the problem of transitions is not encompassed by quantum mechanics in its present form, but that here new conceptual developments will be necessary. I myself, impressed with the closed character of the logical nature of quantum mechanics, came to the presumption that this theory is complete and that the problem of transitions must be contained in it. I believe that I have now succeeded in proving this.

Bohr has already directed attention to the fact that all difficulties of principle associated with the quantum approach which meet us in the emission and absorption of light by atoms also occur in the interaction of atoms at short distances and consequently in collision processes. In collisions one deals not with mysterious wave fields, but exclusively with systems of material particles, subject to the formalism of quantum mechanics. I therefore attack the problem of investigating more closely the interaction of the free particle (α-ray or electron) and an arbitrary atom and of determining whether a description of a collision is not possible within the framework of existing theory.

Of the different forms of the theory only Schrödinger's has proved suitable for this process, and exactly for this reason I might regard it as the deepest formulation of the quantum laws. The course of my reasoning is the following.

If one wishes to calculate quantum mechanically the interaction of two systems,

[†] This report was originally intended for *die Naturwissenschaften*, but could not be accepted there for lack of space. I hope that its publication in this journal [*Zeitschrift für Physik*] does not seem out of place [M.B.].

then, as is well known, one cannot, as in classical mechanics, pick out a state of
the one system and determine how this is influenced by a state of the other system,
since all states of both systems are coupled in a complicated way. This is true also
in an aperiodic process, such as a collision, where a particle, let us say an electron,
comes in from infinity and then goes off to infinity. There is no escape from the
conclusion that, as well before as after collision, when the electron is far enough
away and the coupling is small enough, a definite state must be specifiable for the
atom and likewise a definite rectilinear motion for the electron. The problem is
to formulate mathematically this asymptotic behavior of the coupled particles.
I did not succeed in doing this with the matrix form of quantum mechanics, but
did with the Schrödinger formulation.

According to Schrödinger, the atom in its nth quantum state is a vibration of a
state function of fixed frequency W_n^0/h spread over all of space. In particular, an
electron moving in a straight line is such a vibratory phenomenon which corre-
sponds to a plane wave. When two such waves interact, a complicated vibration
arises. However, one sees immediately that one can determine it through its
asymptotic behavior at infinity. Indeed one has nothing more than a "diffraction
problem" in which an incoming plane wave is refracted or scattered at an atom.
In place of the boundary conditions which one uses in optics for the description
of the diffraction diaphragm, one has here the potential energy of interaction be-
tween the atom and the electron.

The task is clear. We have to solve the Schrödinger wave equation for the
system atom-plus-electron subject to the boundary condition that the solution in
a preselected direction of electron space goes over asymptotically into a plane
wave with exactly this direction of propagation (the arriving electron). In a thus
selected solution we are further interested principally in a behavior of the
"scattered" wave at infinity, for it describes the behavior of the system after the
collision. We spell this out a little further. Let $\psi_1^0(q_k)$, $\psi_2^0(q_k)$, ... be the eigenfunc-
tions of the unperturbed atom (we assume that there is only a discrete spectrum).
The unperturbed electron, in straight-line motion, corresponds to eigenfunctions
$\sin(2\pi/\lambda)(\alpha x + \beta y + \gamma z + \delta)$, a continuous manifold of plane waves. Their wave-
length, according to de Broglie, is connected with the energy of translation τ by
the relation $\tau = h^2/(2\mu\lambda^2)$. The eigenfunction of the unperturbed state in which
the electron arrives from the $+z$ direction, is thus

$$\psi_{n,\tau}^0(q_k, z) = \psi_n^0(q_k) \sin(2\pi z/\lambda).$$

Now let $V(x, y, z; q_k)$ be the potential energy of interaction of the atom and the
electron. One can then show with the help of a simple perturbation calculation
that there is a uniquely determined solution of the Schrödinger equation with a
potential V, which goes over asymptotically for $z \to +\infty$ into the above function.

The question is now how this solution behaves "after the collision."

The calculation gives this result: The scattered wave created by this perturbation has asymptotically at infinity the form:

$$\psi^1_{n\tau}(x, y, z; q_k) = \sum_m \iint_{\alpha x + \beta y + \gamma z > 0} d\omega\, \Phi_{n_\tau m}(\alpha, \beta, \gamma) \sin k_{n_\tau m}(\alpha x + \beta y + \gamma z + \delta)\psi^0_m(q_k).$$

This means that the perturbation, analyzed at infinity, can be regarded as a superposition of solutions of the unperturbed problem. If one calculates the energy belonging to the wavelength $\lambda_{n\tau m}$ according to the de Broglie formula, one finds

$$W_{n_\tau m} = h\nu^0_{nm} + \tau,$$

where the ν^0_{nm} are the frequencies of the unperturbed atom.

If one translates this result into terms of particles, only one interpretation is possible. $\Phi_{n_\tau m}(\alpha, \beta, \gamma)$ gives the probability* for the electron, arriving from the z-direction, to be thrown out into the direction designated by the angles α, β, γ, with the phase change δ. Here its energy τ has increased by one quantum $h\nu^0_{nm}$ at the cost of the energy of the atom (collision of the first kind for $W^0_n < W^0_m$, $h\nu^0_{nm} < 0$; collision of the second kind $W^0_n > W^0_m$, $h\nu^0_{nm} > 0$).

Schrödinger's quantum mechanics therefore gives quite a definite answer to the question of the effect of the collision; but there is no question of any causal description. One gets no answer to the question, "what is the state after the collision," but only to the question, "how probable is a specified outcome of the collision" (where naturally the quantum mechanical energy relation must be fulfilled).

Here the whole problem of determinism comes up. From the standpoint of our quantum mechanics there is no quantity which in any individual case causally fixes the consequence of the collision; but also experimentally we have so far no reason to believe that there are some inner properties of the atom which condition a definite outcome for the collision. Ought we to hope later to discover such properties (like phases or the internal atomic motions) and determine them in individual cases? Or ought we to believe that the agreement of theory and experiment—as to the impossibility of prescribing conditions for a causal evolution—is a pre-established harmony founded on the nonexistence of such conditions? I myself am inclined to give up determinism in the world of atoms. But that is a philosophical question for which physical arguments alone are not decisive.

In practical terms indeterminism is present for experimental as well as for theoretical physicists. The "yield function" Φ so much investigated by experimentalists is now also sharply defined theoretically. One can determine it from the potential energy of interaction, $V(x, y, z; q_k)$. However, the calculations required

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* Addition in proof: More careful consideration shows that the probability is proportional to the square of the quantity $\Phi_{n_\tau m}$.

for this purpose are too complicated to communicate here. I will only clarify briefly the meaning of the function $\Phi_{n,m}$. If, for example, the atom before the collision is in the normal state $n = 1$, then it follows from the equation

$$\tau + hv^0_{1m} = \tau - hv^0_{m1} = W_{1,m} > 0,$$

that, for an electron with less energy than the lowest excitation energy of the atom, the final state is also necessarily $m = 1$, or that $W_{1,1}$ must be equal to τ. Then we have "elastic reflection" of the electron with the yield function $\Phi_{1,1}$. If τ increases beyond the first excitation level, then there occurs, besides reflection, also excitation with the yield $\Phi_{1,2}$, etc. If the target atom is in the excited state $n = 2$ and $\tau < hv^0_{21}$, then there occur reflection with yield $\Phi_{2,2}$ and collisions of the second kind with the yield $\Phi_{2,1}$. If the kinetic energy $\tau > hv^0_{21}$, then further excitation is also possible.

The formulas thus reproduce completely the qualitative character of collisions. The quantitative predictions of the formulas for particular cases require extensive investigation.

I do not exclude the possibility that the strict connection of mechanics and statistics as it comes to light here will demand a revision of basic ideas of thermodynamics and statistical mechanics.

I also believe that the problem of radiation of light—and irradiation—has to be handled in a way entirely analogous to the "boundary value problem" of the wave equation, and will lead to a rational theory of radiation damping and linebreadths in agreement with the theory of light quanta.

An extended treatment will appear shortly in this journal.