The multi-valuedness of the wave function

By Erwin Schrödinger

Translated by D. H. Delphenich

The question arises of whether one is justified in requiring the single-valuedness of the wave function (1). It is only by means of the requirements on wave functions that the eigen-solutions will be distinguished from the other ones to begin with. If one alters the requirements then one will alter the system of eigen-solutions and eigenvalues. That can either eliminate the agreement with experiments or bring it about. One is then not merely dealing with, say, an issue that is intrinsic to the mathematical apparatus.

The wave function is not observable. Hence, one cannot place any demand upon it directly, but only upon the statements that observers might make about it. The values of observable quantities (or more precisely, their probabilities) must be stated uniquely. One can hardly reject, a limine, the possibility of imagining configuration space as being multiplied into a sort of Riemann surface and ascribing several branches to the wave function. However, first of all, the same statements must be true on each branch of a wave function. Secondly, it is probably necessary to demand that for a certain problem that has been presented in a certain way, all wave functions on a certain configuration space that has been multiplied in a certain way can be brought into such a form that one can be able to speak unambiguously of corresponding branches of two different wave functions (which naturally does not exclude the possibility that there are functions among them that coincide in several, or even all, branches).

We first examine the:

1. Scalar wave function

The value of $\psi^* \psi$ at a particular place is mainly observable as the density of the probability that the system will be found in the state in question. Generally, there is an immensely important special case – viz., degeneracy by equal particles – in which there are other places in the (simple) configuration space that correspond to the same state. Strictly speaking, only the sum of the $\psi^* \psi$ at all of those places will then be observable. However, since only the classes of functions that are antisymmetric in all particles actually come under consideration in that case, $\psi^* \psi$ will have the same value at all of the places, and the assertion that it is observable will remain justified.

Now, if $\psi$ and $\chi$ are two branches of a certain wave function then one must have:

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\normalsize
\( \psi^* \psi = \chi^* \chi \).

If we set:
\( \chi = \beta \psi \)
then \( \beta \) must have the form:
\( \beta = e^{i\lambda} \),

with real \( \lambda \), which might be a coordinate function initially, and indeed might perhaps be another one for another pair of branches of the same wave function or the corresponding one or another pair of branches of a different wave function.

Now, suppose that the ratio \( \beta' \) is:
\( \chi' = \beta' \psi' \)

for the corresponding pair of branches of another wave function that we call \( \psi', \chi' \). We superimpose that pair with the first one with numerical factor \( a \), which is a right that one cannot forfeit without abandoning the most intrinsic kernel of wave mechanics. One must then also have:
\( (\psi + a\psi')^* (\psi + a\psi') = (\chi + a\chi')^* (\chi + a\chi') \).

That will give:
\( a \psi'^* \psi' + a \psi^* \psi' = a \chi'^* \chi' + a \chi^* \chi' \).

If one first takes \( a = 1 \) and then \( a = i \) then it will follow that:
\( \psi'^* \psi + \psi \psi' = \chi'^* \chi + \chi \chi' \),
\( \psi'^* \psi - \psi \psi' = \chi'^* \chi - \chi \chi' \)
so
\( \psi^* \psi' = \chi^* \chi' \),
or, from (4) and (2):
\( \psi^* \psi' = \beta^* \beta' \psi^* \psi' \).

One must then have either:
\( \beta' = (\beta^*)^{-1} = e^{i\lambda} = \beta \)
or
\( \psi \psi' = 0 \).

The second alternative does not prevent one from stating that in general:
\( \beta' = \beta \).

The same ratio will be valid for all wave functions at a particular place for a certain pair of branches.

Hence, the same thing will also be true for the complex conjugate (to the extent that one must allow it, from which, it will follow directly). Now, \( \beta \) will then go to its complex conjugate. The latter must be equal to the former, so it must be real. Hence, it can be only \(+1\) or \(−1\). Therefore, in no event can it have more than two different branches, and since the ratio at a certain place must be the same for all wave functions,
since it cannot jump under continuous variation of the place, moreover, it must follow that:

*One must admit either nothing but single-valued wave functions or nothing but two-valued ones with the modulus $-1$. There is no third possibility. I find no grounds for excluding either of those two possibilities.*

Two premises in the latter proposition require further explanation:

1. Must we really admit the complex conjugate of any wave function? (We mean the complete wave function; i.e., including all of its branches.)

There should be no logical obligation to do that. Generally, there is a complete symmetry between the two square roots of $-1$. A physical theory that uses those symbols in any different way will misuse them. However, $\sqrt{-1}$ appears in the foundation of wave mechanics in the definition of the energy and impulse operators. If one defines, e.g., the energy to be $-\frac{\hbar}{2\pi} \frac{d}{dt}$ (as usual) then now, for example, the function $x + iy$ can be something essentially different from $x - iy$ and can have other properties or rights. Up to now (as far as I know), no one has ever given any sort of significance to the *sign* in the first definition. If one did do that then one would eliminate the temporal reversibility of wave mechanics. I shall content myself by establishing that: The result above will be guaranteed as long as one insists upon the temporal reversibility of wave mechanics, as has always been the case.

2. We said that the ratio cannot have any jumps.

That conclusion is unavoidable when the configuration space is a continuum. That will be true for any “natural” choice of coordinates that is taken from classical mechanics. If one would like to reason on the basis of the *Dirac-Jordan* theory of transformations – i.e., to employ the eigenvalues of an arbitrary complete observable as the coordinate space – then one must reckon with the possibility of discontinuities. (I said “possibility.” One will, in fact, not know the eigenvalues before one is clear about which requirements must be placed upon the wave function.) In that case, the argument will become more complicated, but the result will remain the same. In addition to the probability of presence, one must bring other observables under consideration whose matrix elements link the components of configuration space together, between which, no continuous transition is possible. The treatment of the Dirac electron that is given in section 2 might suffice as a model for such an argument.

2. *The Dirac wave function*

A special examination is desirable of the question of whether or not one can formally interpret ordinary wave functions when the configuration space has been extended by a variable in the domain of definition $(1, 2, 3, 4)$ on the following grounds:
First of all, the squares of the magnitudes of the individual $\psi_k^* \psi_k$ (i.e., not summed!) will correspond to that conception, and one must ponder their fundamental observability for at least a moment. Secondly, the modulus can possibly jump in a discontinuous domain, such as the one that is present here. A third point is the admissibility of complex-conjugate functions. One must then deliberate upon whether things actually still happen as they did for scalar functions.

In order to establish the simple results of the previous section for Dirac functions, as well, the observables of “probability of presence” or “particle density,” which correspond to the identity matrix in spin space, will not suffice, but one must focus on the most general observable, at least, in regard to spin, which will be represented by an arbitrary Hermitian four-matrix \(^{(1)}\).

Let $\alpha_{\rho\sigma}$ be one of them, so one must impose the demand:

\[
\sum_{\rho} \sum_{\sigma} \psi^*_{\rho} \alpha_{\rho\sigma} \psi_{\sigma} = \sum_{\rho} \sum_{\sigma} \chi^*_{\rho} \alpha_{\rho\sigma} \chi_{\sigma}
\]

on the pair of branches $\psi_{\rho}, \chi_{\rho}$ ($r, s = 1, 2, 3, 4$). If one takes just $\alpha_{11} \neq 0$ and all other $\alpha_{\rho\sigma} = 0$ here then it will follow that:

$\psi_i^* \psi_i = \chi_i^* \chi_i$.

One must then have:

$\chi_1 = \beta_1 \psi_1$ \hspace{1em} with $\beta_1 = e^{i\lambda_1}, \lambda_1 \text{ real.}$

(In the event that $\psi_1$ should vanish, $\chi_1$ must also vanish, so the statement will not become false.) Corresponding statements will be true for the second, third, and fourth components, but the four numbers $\beta_k (\lambda_k, \text{ resp.})$ can still be different, to begin with. One will then deduce that they must all be equal (might, resp., in case the components vanish) when one chooses a matrix for $\alpha$ in which, e.g., only $\alpha_{12}$ and $\alpha_{21}$ are non-zero (and complex-conjugate), etc. One will then get (while omitting the spin index):

\[
\chi = \beta \psi, \quad \beta = e^{i\lambda}.
\]

$\lambda$ is a real number that is, however, valid only provisionally for this pair of branches of this wave function at this location in the continuum.

Now, let $\psi', \chi'$ be the corresponding pair of branches of another wave function at the same place, and let:

\[
\chi' = \beta' \psi'.
\]

We shall once more consider the wave function that arises when one superimposes the first one with the second one, multiplied by the number $a$; hence, the one whose

\[^{(1)}\text{Eight of the 16 matrices have immediate physical meanings. They are: The identity, the six velocity-spin components, and the product of a velocity component with the spin component that is parallel to it. One will get the other eight when one multiplies the first eight by the matrix of the mass term, which will keep its somewhat-complicated physical sense in such a way that the remaining parts of the Dirac equation will have one, too.}\]
corresponding pair of branches are $\psi + a\psi', \chi + a\chi'$. For that, we write down the requirement (6), then first set $a = 1$ and then set $a = i$, and easily find that:

$$\sum_\rho \sum_\sigma \psi_\rho^* \alpha_{\rho\sigma} \psi'_\sigma = \sum_\rho \sum_\sigma \chi_\rho^* \alpha_{\rho\sigma} \chi'_\sigma.$$  

What we would like to prove is that either one must set $\beta' = \beta$ or one might demand that, which is trivially the case when all of the components of only one of the two functions vanish at the place in question. We might then assume that, e.g., $\psi_\rho$ (and then naturally $\chi_\rho$, as well), and $\psi'_\sigma$ (and then naturally $\chi'_\sigma$, as well) will vanish at the place. One will then choose the matrix $\alpha$ such that only $\alpha_{\rho\sigma} = \alpha_{\rho\sigma}^*$ is non-zero, and indeed will be equal to 1 once, in any case, and in the case of $\rho \neq \sigma$, it will be equal to $i$ a second time. That will then imply that:

$$\beta^* \beta' = 1, \quad \text{i.e.} \quad \beta' = \beta.$$  

The corresponding pair of branches of all wave functions must all have the same modulus at the same place in the continuum.

One now sees that the further conclusions proceed as they did for scalar functions in the previous section if some need exists to admit the complex-conjugate of a wave function along with that wave function. One would then need to have $\beta = \beta^*$, hence, it would be real, and therefore $+1$ or $-1$. Since it cannot have any jumps under continuous variation of the place in the continuum, for a particular representation, one can have either only single-valued wave functions or only two-valued ones, with a change of sign, which is exactly as before.

Statements that are similar to the ones in number 1 can be made about the need to admit complex-conjugates. The $\sqrt{-1}$ now appears in the energy-impulse operator, as well as in the velocity-spin matrices. However, that will change little. As long as a unique symbol for $\sqrt{-1}$ is introduced into the basic definitions, the choice of a function over its complex-conjugate is indeed basically possible. However, that would mean that one would have to abandon reversibility (due to the energy operator). It is perhaps quite good to know that the present examination also needs to be revised in this case. The purely academic pursuit of that question will have little appeal, however.

I was led to the arguments that were communicated here by the fact that I was recently compelled informally to give a representation of Dirac’s theory in spherical space that would give the correct eigenvalues only for hydrogen atoms when one decides in favor of the alternating solutions, as opposed to the single-valued ones. (The paper will appear in the session reports of the Papal Academy of Science.) It then seems worthwhile to me to work out a theory that at least leads to one alternative, and not to the doubling of the system of eigenvalues that Eddington occasionally feared. It does not
escape me that another theory is also possible, namely, this one: If the configuration space has been multiplied into a kind of Riemann surface then the operators will also conceivably need to be changed, namely, in such a way that the probability of presence will be given, not by the value of $\psi^* \psi$ on one sheet, but by the sum of those quantities over the homologous places on all sheets.

All of our conclusions will need to be proved again with that conception of things. However, lacking that, one recognizes that single-valued and alternating functions will remain admissible in any case, but they will no longer define incompatible function classes, but merely non-combining ones.

That would be somewhat less satisfying. In addition, it seems to me that one would therefore not arrive at the restriction to merely two possibilities.

Summary

The idea will be established that for any particular problem in a particular representation in wave mechanics, one might allow either only single-valued wave functions or only two-valued ones whose two branches differ by only the sign. The admission of the one class will exclude the admission of the other one, and vice-versa.

Graz, Merangasse 20.

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