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Single-Valued and Multi-Valued Schrödinger Wave Functions

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Abstract. We re-examine the question of whether wave functions are always single-valued in non-relativistic quantum mechanics. We find that a general proof of the single-valuedness has so far been given only for cases of high spatial symmetry. (In particular we show that the derivations of the single-valuedness for wave functions describing an Aharonov–Bohm effect appearing in the literature are unsatisfactory.) In this article we prove that the majority of non-relativistic, time-independent wave functions are in fact either single-valued, or multi-valued in such a way that they are unitarily equivalent to single-valued functions. This result is a direct consequence of the ellipticity of the Schrödinger equation and of the simply-connectedness of the three-dimensional Euclidian space. Therefore no special postulate is required to guarantee the single-valuedness of non-relativistic wave functions.

1. Introduction

In non-relativistic quantum mechanics it is often assumed that wave functions are or must be chosen single-valued. This assumption is sometimes used to prove the fundamental result that the canonical orbital angular momentum is integer [1]. The single-valuedness assumption further plays a decisive role in the theory of systems showing enclosed magnetic flux (Josephson effect [2], trapped magnetic flux in superconductors [3–10], magnetic Aharonov–Bohm effect [see e.g. 11–19]).

It is well known (see e.g. [20]) that the single-valuedness does not follow from basic quantum mechanical postulates and that a certain kind of multi-valued (i.e. path dependent) wave functions cannot be excluded *a priori*. Therefore the question arises whether the single-valuedness assumption of non-relativistic quantum mechanics is at all correct and, if so, what is its correct theoretical justification (in particular: does it follow from the Schrödinger equation or only from an additional postulate?).

In Section 2 we give a critical review of the literature on this subject which reveals that the treatment of these questions has been incomplete and partly incorrect. We shall see that a correct proof of the single-valuedness of the Schrödinger function in general has so far been given only in cases of very high spatial symmetry and, further, that the question of single-valuedness is sometimes not clearly distinguished from the question why orbital angular momenta are integer and from the special aspects of Hamiltonians which are defined in multiply connected regions.

In this paper we shall clarify these subjects. In particular we shall be able to show that the usual Schrödinger functions (including those describing a system with enclosed

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magnetic flux) are in fact single-valued (apart from possible multi-valued unitary transformations), and that this is a direct consequence of the mathematical structure of the Schrödinger equation of the considered physical system (Sections 3 and 4).

2. Critical Review of the Literature

In an older article Pauli [20] suggests a general criterion by which one could answer the question of whether wave functions are single-valued or multi-valued. His criterion is equivalent (cf. [16]) to the property of wave functions to provide a basis for a representation of the symmetry group of the Hamiltonian. How the single-valuedness may follow from this property is best illustrated by an example: Consider a spherically symmetric, spinless one-particle Hamiltonian. Here a Schrödinger function $\psi(\mathbf{r})$ (which belongs to a finite-dimensional eigenspace) is a finite sum of functions of the form $R(r)\cdot f(\theta,\varphi)$, where $f(\theta,\varphi)$ is square integrable on the unit sphere and transforms according to a representation of the three-dimensional rotation group. Since the basis functions for such a representation of the rotation group are known from group theory to be single-valued on each sphere around the center of co-ordinates ([21], chapt. 15), it follows that $R(r)\cdot f(\theta,\varphi)$, and hence $\psi(\mathbf{r})$ are single-valued in R^3 (provided $R(r)$ is single-valued).

From this example it is easy to see that the proof of the single-valuedness of the total Schrödinger function by group theoretical considerations is restricted essentially to spherically symmetric Hamiltonians and that this method fails in cases of little or no spatial symmetry. Nevertheless it appears to be the only correct method which has been used in the literature to prove the total or partial (e.g. around an axis) single-valuedness of Schrödinger functions (cf. [16]). We emphasize that this method of proof derives the single-valuedness from the Schrödinger equation and not from an additional postulate.

There exist other derivations of the single-valuedness, which are based on the fact that orbital angular momenta are integer [22; 14, 17, 18, 23; cf. 8–10]. They do, however, not provide a real proof since they are based on additional postulates. In fact, we cannot derive properties of Schrödinger functions from given properties of orbital angular momentum operators since these operators alone are in a certain sense arbitrary and are only fully determined by the very Schrödinger equation (and its solutions) of the particular physical system under consideration. As an illustration take the operator of the z-component of the canonical orbital angular momentum

$$L_z = -i\hbar\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right) = -i\hbar\frac{\partial}{\partial\varphi} \tag{1}$$

(φ is the angle of rotation around the z-axis). This operator, considered as a self-adjoint operator in the space $\mathscr{L}_2(R^3)$ of square integrable functions, is not fully defined. It can be shown [23] that L_z admits a whole family of self-adjoint extensions, each of which is determined by a boundary condition

$$\lim_{\epsilon\to 0}\psi(r,\theta,2\pi-\epsilon) = e^{i2\pi(a+m)}\psi(r,\theta,0), \tag{2}$$

which itself is characterized by the real number a, $0 \leqslant a < 1$ (m is an arbitrary integer). Now, in physics, we cannot speak of an angular momentum of itself but only of the angular momentum of a particular physical system, which in turn is fully described by its Schrödinger equation. Hence a wave function $\psi(\mathbf{r})$ which describes a sharp orbital

angular momentum of the system is not only an eigenfunction of L_z but also a solution of the Schrödinger equation of that system. This is a restrictive condition on the domain of definition of L_z, which determines a definite self-adjoint extension of L_z. For instance, take a Schrödinger equation which admits only single-valued solutions, or which is invariant under rotations around the z-axis whence according to group theoretical considerations its solutions are single-valued around the z-axis. Here the parameter a in (2) becomes zero.

Reference [23] leans on two articles [24, 25] where the fact that orbital angular momenta are integer is derived, as it is claimed, from the formal theory of angular momenta, i.e., without making use of a property of a Schrödinger equation (e.g., of a transformation group). However, a careful reading of these articles shows that such a property is hidden in the assumptions: in [24] the fulfilment of Pauli's criterion with respect to the spherical group is contained in assumption No. 3, and in [25] the same assumption is made implicitly by representing the orbital angular momentum operators as matrices, which is only possible for those self-adjoint extensions whose eigenfunctions transform according to the spherical group (see [16, 20]).

3. A Sufficient Condition for the Single-Valuedness of Schrödinger Functions

We consider a system of N particles (charges q_k, masses m_k, $k = 1, 2, \ldots, N$) situated in a *simply connected* region g of the three-dimensional Euclidian space R^3. The corresponding spin-free, time-independent Schrödinger equation reads

$$H\psi(x) = E\psi(x), \quad x \in G \subset R^{3N}. \tag{3}$$

Here G is the N-fold Cartesian product of g and hence a simply connected region in the $3N$-dimensional space R^{3N}, and

$$x = (x_1, x_2, \ldots, x_{3N}) = (\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N)$$

is the position vector in the space R^{3N}. The Hamiltonian has the general form

$$\begin{aligned} H &= \sum_{\alpha=1}^{3N} a(x)\left(\frac{\partial}{\partial x_\alpha}\right)^2 + b_\alpha(x)\frac{\partial}{\partial x_\alpha} + c(x) \\ &= \sum_{k=1}^{N} (1/2m_k)\left\{(\hbar/i)\frac{\partial}{\partial \mathbf{r}_k} + (-q_k/c)\mathbf{A}(\mathbf{r}_k)\right\}^2 + V(x), \end{aligned} \tag{4}$$

where $\mathbf{A}(\mathbf{r})$ is the magnetic vector potential due to an external magnetic field $\mathbf{B}(\mathbf{r})$, $V(x)$ is the electrostatic potential of the (internal or external) electric field, and c is the velocity of light.

Quantum mechanics requires the Hamiltonian H to be an operator in the complex Hilbert space $\mathscr{L}_2(G)$ of square integrable functions on G. For the following we further use the fact that the differential operator H is elliptic[2]) in R^{3N}. This property enables us to apply a regularity theorem [26] for elliptic differential operators, which gives us information about the analytic behaviour of the $\mathscr{L}_2(G)$-eigensolutions $\psi(x)$ of H in function of the regularity of the potentials $\mathbf{A}(\mathbf{r})$ and $V(x)$. Let S be the set of all points x of G where the coefficients $a(x)$, $b_\alpha(x)$, $c(x)$ of the differential operator H are not analytic in R^{3N} [27]. It immediately follows [28] from the quoted theorem that all the solutions of (3) are analytic in $G - S$.

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[2]) For a definition see [26], p. 75, definition 3.3.2.

We now consider the case where the set $G - S$ is simply connected in R^{3N}. Then it follows from the analyticity that all the eigenfunctions $\psi(x)$ of the Hamiltonian H are single-valued in $G - S$. The proof is analogous to the proof of the corresponding theorem [29] for functions of one complex variable. (One has to use the fact that the properties of analytic functions of one complex variable which are used in the quoted proof also hold for analytic functions of several real variables (cf. [27]).

Definition We say that a Hamiltonian of type (4) has the property A, if in addition to $G - S$ being simply connected the set S is of Lebesgue measure zero in R^{3N}. If this occurs the solution $\psi(x)$ is equivalent to a function which is also single-valued on S since we consider $\mathscr{L}_2(G)$-solutions of (3). Therefore we may say that in this case any eigenfunction of the Hamiltonian (4) is single-valued in the whole domain G. Thus the property A is a sufficient condition for a Hamiltonian of type (4) to have only single-valued eigenfunctions. We emphasize that this condition is not restricted to a special class of symmetries.

We observe that a large number of physically meaningful Hamiltonians has the property A. Consider e.g. a system of charged particles in a region where there is no external magnetic field, and where the electric potential function $V(x)$ represents the Coulomb interactions of the particles among themselves and the Coulomb interactions with external, fixed point charges (as in the usual non-relativistic Born–Oppenheimer Hamiltonian for molecular systems). Here S is the union of $(3N-3)$-dimensional manifolds in R^{3N}. Hence S is of measure zero, and $G - S$ is simply connected in R^{3N}.

Moreover, the majority of external potentials other than Coulomb potentials are polynomials or exponential functions with the property A[3]) (e.g. potentials of a homogeneous electric field, of harmonic and anharmonic oscillators, or of Morse type). Quite generally it appears that any reasonable electric potential either has the property A or can be approximated by such a potential. In addition, also many magnetic vector potentials have the property A (e.g. consider a homogeneous field, where $\mathbf{A}(\mathbf{r}) = \frac{1}{2}\mathbf{B}\times\mathbf{r}$, or a dipolfield, where $\mathbf{A}(\mathbf{r}) = \boldsymbol{\mu}\times\mathbf{r}/r^3$).

4. Hamiltonians Which do not Have the Property A

If the Hamiltonian does not have the property A, or if the group theoretical method described in Section 2 is not applicable, additional methods are needed in order to find out whether the Schrödinger functions are single-valued or multi-valued. We discuss three typical examples.

a) *Multi-valued Schrödinger functions generated by unitary transformations*

Consider the Hamiltonian

$$H = (1/2m)\sum_{\alpha=1}^{3N}\left\{(\hbar/i)\frac{\partial}{\partial x_\alpha} + (-q/c)\mathscr{A}_\alpha(x) + \frac{\partial}{\partial x_\alpha}F(x)\right\}^2 + V(x), \tag{5}$$

defined in the Hilbert space $\mathscr{L}_2(R^3)$. (For simplicity we take N identical particles.) Here $\mathscr{A}_\alpha(x)$ is the α-th component of the $3N$-dimensional vector $(\mathbf{A}(\mathbf{r}_1), \mathbf{A}(\mathbf{r}_2), \ldots,$

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[3]) A function $f(x)$ has the property A if the set S' where $f(x)$ is not analytic is of measure zero, and $G - S'$ is a simply connected region. If the potential functions $V(x)$, $A_\alpha(r)$, $\alpha = 1, 2, 3$, have the property A, then clearly the Hamiltonian has this property as well.

$\mathbf{A}(\mathbf{r}_N)$), where $\mathbf{A}(\mathbf{r})$ is the vector potential of the external magnetic field. The corresponding Schrödinger equation is equivalent to $H'\psi'(x) = E\psi'(x)$, where

$$H' = (1/2m)\sum_{\alpha=1}^{3N}\left\{(\hbar/i)\frac{\partial}{\partial x_\alpha} + (-q/c)\mathscr{A}_\alpha(x)\right\}^2 + V(x) \tag{6}$$

and

$$\psi'(x) = \psi(x)\cdot e^{(i/\hbar)F(x)}.$$

The physical quantities are independent of the special form of the function $F(x)$ even if $F(x)$ is multi-valued around one or several $(3N-2)$-dimensional hypersurfaces Σ_k. In this latter case the Hamiltonian H does not have the property A because of the singularity of $(\partial/\partial x_\alpha)F(x)$ on the $(3N-2)$-dimensional hypersurfaces Σ_k.

Now let us consider the case where (6) has only single-valued solutions (e.g., take H such that H' has the property A). As a consequence the solutions $\psi(x) = \psi'(x)\cdot e^{-(i/\hbar)F(x)}$ of the original Schrödinger equation (5) are multi-valued along any closed path P_k in in R^{3N} which once encircles the hypersurface Σ_k (provided

$$(1/2\pi\hbar)\oint_{P_k}\frac{\partial}{\partial x_\alpha}F(x)dx_\alpha$$

is not an integer).

Therefore, and since (5) and (6) are physically equivalent, the question of single-valuedness for Schrödinger functions actually reads: does the class of unitarily equivalent Hamiltonians of a considered physical system contain at least one representative which has only single-valued eigenfunctions?

b) *Systems showing enclosed magnetic flux* (cf. Section 4c)

Consider an electron in an external electromagnetic field such that the magnetic field is confined to an infinitely long cylinder V_c with radius R_2 (centered by the z-axis). The vector potential of such a system does not have the property A. Nevertheless it can be proved that the Schrödinger functions are single-valued by using our method of Section 3 together with an additional regularity theorem for elliptic operators of Schrödinger type of the sort as stated, e.g. in [30].

As a concrete example we consider a vector potential $\mathbf{A}(\mathbf{r})$ for which A_z and the radial component A_r are zero and the angular component A_φ takes the values

$$\begin{aligned} A_\varphi(r) &= Br/2 \quad \text{for } r \leqslant R_1 \quad (0 < R_1 < R_2) \\ &= \phi/2\pi r \quad \text{for } r \geqslant R_2 \\ &= P(r) \quad \text{for } R_1 \leqslant r \leqslant R_2, \end{aligned}$$

where $P(r)$ is a third-order polynomial in r such that $A_\varphi(r)$ and its first-order derivative are continuous at $r = R_1$ and $r = R_2$ (such a polynom always exists). Here φ is the angle of rotation around the z-axis, and ϕ is the total magnetic flux contained in the cylinder V_c. The cartesian components of this vector potential are analytic in R^3 except on the two surfaces $r = R_1$ and $r = R_2$, where they are only continuously differentiable. Further we consider an electric potential $V(r)$ which has the property A in R^3, and whose

singularities are of Coulomb type[4]). We now can apply the supplement to Theorem 3.2 of [30], from which it follows that the Schrödinger functions $\psi(\mathbf{r})$ are continuous at $r = R_1$ and $r = R_2$. Further, from the property A of the Hamiltonian inside the cylinder $C_1 = \{r|0 \leqslant r < R_1\}$ together with the continuity of $\psi(\mathbf{r})$ on its boundary $(r = R_1)$ it follows that $\psi(\mathbf{r})$ is single-valued in the closed cylinder $\bar{C}_1$ $(r \leqslant R_1)$. In an analogous way one proves that $\psi(\mathbf{r})$ is single-valued along any closed path which is contained in the closed hollow cylinder $\bar{C}_2 = \{r|R_1 \leqslant r \leqslant R_2\}$, but which does not encircle the z-axis. This property in turn guarantees that the change of a particular function $\psi(\mathbf{r})$ along a closed path which in $\bar{C}_2$ encircles once the z-axis is the same for all such paths. From the single-valuedness of $\psi(\mathbf{r})$ along such a path lying entirely on the boundary $(r = R_1)$ of $\bar{C}_1$, and from the continuity of $\psi(\mathbf{r})$ it follows that $\psi(\mathbf{r})$ is single-valued in the union of $\bar{C}_1$ and $\bar{C}_2$. Finally, in a similar way the proof of the single-valuedness of $\psi(\mathbf{r})$ is extended to the whole space R^3.

In the limit where R_2 tends to zero but ϕ remains finite, our Hamiltonian formally looks like an operator of type (5) with $F(\mathbf{r})$ multi-valued around the z-axis $(N = 1)$. However, we emphasize that this limit operator has a domain of definition in $\mathscr{L}_2(R^3)$ which is different from the one belonging to the formally corresponding operator of type (5). It therefore cannot be generated by a unitary transformation (formal gauge transformation using $F(\mathbf{r})$) from a Hamiltonian which describes a particle in the absence of a magnetic field.

c) *Multiply connected regions*

The questions of single-valuedness and multi-valuedness have been raised especially in connexion with Schrödinger equations which are defined in multiply connected regions. For a discussion of such equations the following general remarks are useful. Quantum mechanics requires the Hamiltonian to be essentially self-adjoint in the Hilbert space $\mathscr{L}_2(G)$ (cf. [31]). It has been shown [31, 32] that for a very large class of electromagnetic potentials, including Coulomb potentials, the Hamiltonian (4) in fact is essentially self-adjoint, provided the domain of definition G is simply connected. If G is multiply connected the Hamiltonian is no longer essentially self-adjoint and hence the Schrödinger equation is not completely defined. Consider for instance a particle which is contained in a doubly connected region, e.g. the region outside an infinitely long cylinder. In this case there exists a one-parameter family of self-adjoint extensions of H, each of which is determined by a circulation boundary condition analogous to (2) [19]. We remark that all except one of these extensions have multi-valued eigenfunctions. This means that here, from a pure mathematical point of view, we do have a choice between single-valued and multi-valued eigenfunctions. Physically however only one of these extensions is correct, which now has to be determined. (Compare Section 2, where we had to determine the physically correct self-adjoint extension of L_z.) This can be achieved by making the Schrödinger equation of the multiply connected region consistent with a covering Schrödinger equation which is defined in a simply connected region containing the multiply connected region, and which is therefore completely defined. (We remark that a Schrödinger equation defined in a multiply connected region is always an approximation or restriction of such a covering theory.)

As an example we consider a charged particle in the space R^3, which is subject to an electromagnetic potential which has the property A, or which is of the type discussed in Section 4b) and whose form is such that the modulus of any Schrödinger function of the

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[4]) Under these conditions the Hamiltonian is essentially self-adjoint in $\mathscr{L}_2(R^3)$ [30].

system is negligible within a volume V_c, shaped as a torus or as an infinitely long cylinder. This one-particle system may be approximately described by a Schrödinger equation

$$H_a \psi_a(\mathbf{r}) = E_a \psi_a(\mathbf{r}) \tag{7}$$

to be solved in the doubly connected region $g = R^3 - V_c$, with the boundary condition $\psi_a(\mathbf{r}) = 0$ at the boundary of V_c. Now the covering theory, given by the Schrödinger equation defined in the whole space R^3, admits only single-valued solutions, which follows according to Sections 3 and 4b) without solving the equation. Hence the approximate equation (7) must be solved with the subsidiary condition that its solutions be single-valued. This condition uniquely determines the physically correct self-adjoint extension of the Hamiltonian H_a.

In the theories of the Aharonov–Bohm effect and of trapped magnetic flux one usually considers such an approximate Schrödinger equation of type (7). However, the determination of a definite self-adjoint extension of the Hamiltonian H_a is not derived from a covering equation defined in the whole space R^3 as it should, but is based on the requirement that the functions $\psi_a(\mathbf{r})$ have to be single-valued [3–10, 12, 13, 15, 16, 19] or that the canonical orbital angular momentum operator L_z must have integer eigenvalues [14, 18, cf. 8–10, 17, 23]. These derivations are unsatisfactory since they introduce additional postulates (cf. Section 2).

Final Remark

We have shown that the time-independent Schrödinger functions are in fact single-valued (apart from possible unitary transformations), and that this is a direct consequence of the ellipticity of the Schrödinger equation. (No new quantum mechanical postulate is required.) This result may be considered as a starting point for future investigations searching for physically significant multi-valued wave functions, since it indicates that such wave functions cannot be solutions of wave equations of elliptic type.

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