

CONSEQUENCES OF NONSEPARABILITY OF QUANTUM MECHANICAL WAVE FUNCTIONS

ELIAHU COMAY

*Raymond and Beverly Sackler Faculty of Exact Sciences,
School of Physics and Astronomy, Tel Aviv University, Tel Aviv 69978, Israel*

Received 20 April 1987

UDC 530.182

Original scientific paper

An analysis based upon fundamental properties of quantum mechanics shows that the electric Aharonov-Bohm effect does not exist. This conclusion is not incompatible with experiment. The significance of the nonseparable nature of quantum mechanical wave functions is discussed.

1. Introduction

The Aharonov-Bohm (AB) effects^{1,2)} analyse the interference pattern of a split wave function of a charge moving in a nonsimply connected field-free region of space. Introducing the potential associated with an inaccessible electromagnetic field, the effects predict a finite phase shift of the interfering charge. The two kinds of the AB effect are distinguished according to whether an electric or a magnetic field is associated with the potential variation.

These effects are considered a controversial issue for a very long time³⁻⁷⁾. By contrast, the general acceptability of other quantum mechanical predictions indicate the peculiar status of the AB effects. The present work discusses the electric AB effect and no claim is made concerning its magnetic version. The electric AB effect lacks two basic supports required for establishing a physical effect: it has never been confirmed experimentally^{6,7)} and, as shown recently⁷⁾, its original derivation is wrong. The present work goes one step further. Relying upon basic properties of quantum mechanics, it proves that the electric version of the AB effect does not exist at all.

The significance of the mathematical form of wave functions describing quantum mechanical systems of several particles is analysed. It is well known that the wave function of a system of two different particles that have never interacted in the past can be written in a multiplicative form

$$\Psi = \Phi(\vec{r}_1, t) \psi(\vec{r}_2, t). \quad (1)$$

In the case of two identical fermions, the right hand side of this expression is written as a single Slater determinant. This latter form of wave functions is put here together with (1) in the same category. Henceforth, the term *multiplicative* denotes this category of wave functions.

On the other hand, a system of two different particles that have interacted in the past cannot generally take the multiplicative form. For a system of this kind, the following expression is used

$$\Psi = \sum_{i,j} a_{ij} \Phi_i(\vec{r}_1, t) \psi_j(\vec{r}_2, t). \quad (2)$$

The corresponding expression for two identical fermions is a linear combination of Slater determinants. Henceforth, the term *nonseparable* denotes this kind of wave functions.

Two examples of the significance of the nonseparable nature of quantum mechanical wave functions are discussed. The second section of this work is devoted to a comparison of two calculations of the ground state of the Be atom. It shows that the nonseparable approach, which uses a linear combination of many Slater determinants, yields very accurate results while a utilization of a single determinant serves as an approximation. The third section presents the main point of this article. It discusses the electric version of the *AB* effect^{1,2}). The original derivation of the electric effect uses a wave function that takes a multiplicative form³). On the other hand, an examination of a nonseparable wave function, carried out in the third section, proves that the effect disappears. Several conclusions are the contents of the last section.

2. An atomic energy level

Two different calculations of the ground state of the Be atom illustrate the degree of accuracy of a multiplicative wave function⁸⁾ and that of a nonseparable one⁹⁾. The multiplicative approach uses a Hartree-Fock self-consistent wave function of a single configuration $1s^2 2s^2$. The calculation based on a nonseparable wave function uses many different configurations. Several results of these calculations are presented on Table 1.

The first line of this table shows the final value obtained from a multiplicative wave function that uses a single configuration. The next three lines contain results

of the nonseparable approach. The second line presents the nonrelativistic interaction obtained from 697 configurations. A successive increase of the dimension of

TABLE 1.

Method	E/H
Hartree-Fock,	—14.57434
697 configurations ^a	—14.66690285
∞ configurations ^b	—14.666921(2)
inclusion of relativity ^b	—14.669344(25)
experiment ^c	—14.669345(2)

Energy level of the ground state of the Be atom ($1H = 4.36 \cdot 10^{-18}$ J).

^a Ref. 8, p. 121.

^b Ref. 9, Table VIII.

^c Ref. 9, Table X.

the Hilbert subspace shows the dependence of the result on the number of configurations used. The third line of the table contains the value obtained from an extrapolation to an infinite number of configurations. The addition of relativistic corrections as well as of some minor nonrelativistic ones yields the final result of the nonseparable approach. It is written on the fourth line of the table.

These values can be compared with the experimental quantity which is written on the last line of the table. It is found that the result of the nonseparable approach is very accurate. The relative accuracy of the multiplicative approach is worse. It is also well known that the binding energy obtained from a calculation that uses a subspace of the entire Hilbert space is smaller than the accurate value. This property, which can also be seen in Table 1, shows that the multiplicative approach lacks the contributions obtained from many other configurations that are not included in it.

On the other hand, the results of the multiplicative approach are of a highly important value. It is shown that the binding energy of the Be atom is found with an inaccuracy of less than one percent. It should also be noted that this approach yields results for any atom⁸⁾. On the other hand, calculational problems of the nonseparable approach make the computation of an energy level of a many electron atom very difficult. Hence, for most atoms, the multiplicative approach is an important practical method that provides calculated values of atomic energy levels.

The foregoing discussion can be concluded as follows. The nonseparable approach, which is based upon basic properties of quantum mechanics, yields accurate results. On the other hand, the application of a multiplicative wave function, which relies upon the atomic shell model, provides approximate values. This is an example of the (relatively) accurate nature of a good theory and of the approximations inherent even in a good model. The benefits of a good model are also demonstrated in this case. Indeed, the atomic shell model satisfies two requirements: the energy levels obtained are rather good and the calculations involved are much simpler.

3. The electric Aharonov-Bohm effect

An analysis of the electric AB effect is the subject of this section. The original presentation of this effect^{1,2)} uses a chopped beam of electrons that is split coherently into two wave packets. The following experiment is designed to test this effect (see Fig. 1). Henceforth, the electron described by the two subpackets is called *the moving electron*.

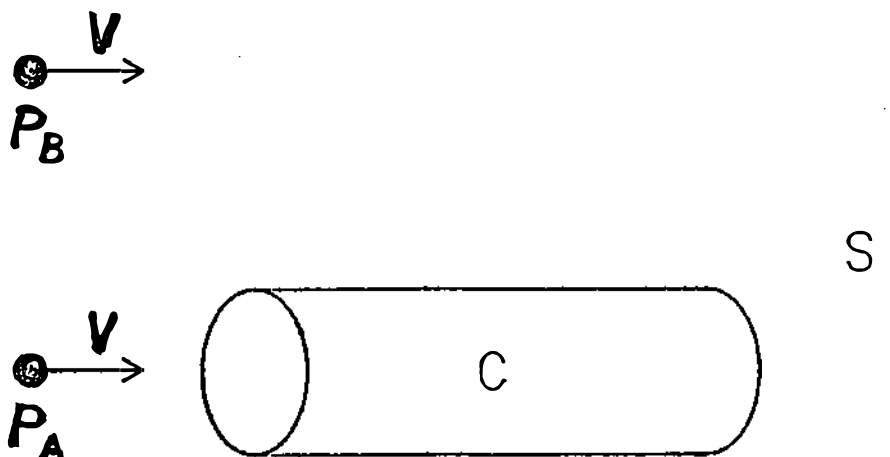


Fig. 1. Two coherent wave packets of a single electron, P_A and P_B , move from left to right. P_A runs through a long hollow cylinder C and P_B runs at its outer side. Later, the two wave packets interfere on the screen S .

The cylinder consists of two layers which are made of insulating materials. The inner rigid layer is covered uniformly with positive charges and the outer flexible layer is analogously covered with the same amount of negative charges. Before P_A enters the cylinder, the distance between its two layers is infinitesimal and the electrostatic potential associated with their charges vanishes everywhere. Later, when P_A is well inside the cylinder, a special regulator releases a fixed amount of energy and pushes adiabatically the flexible layer in a radial direction in a manner that keeps its cylindrical shape. The inflated flexible layer stays motionless for a short time after which it returns adiabatically to its original size. This motion terminates while the moving electron is still far from the cylindrical ends (see Fig. 2). After leaving the cylinder, the two wave packets interfere on the screen S . The interference pattern obtained in this experiment is compared with that of a null experiment where the cylinder is motionless and its potential vanishes identically. It is assumed that all the charges move slowly and that the nonrelativistic limit holds.

The first presentation of the effect¹⁾ uses a single particle wave function of the moving electron. This approach is unsatisfactory because the constituents of the system interact with each other and the self energy of the potential source varies during the process. This approach is not discussed here any more.

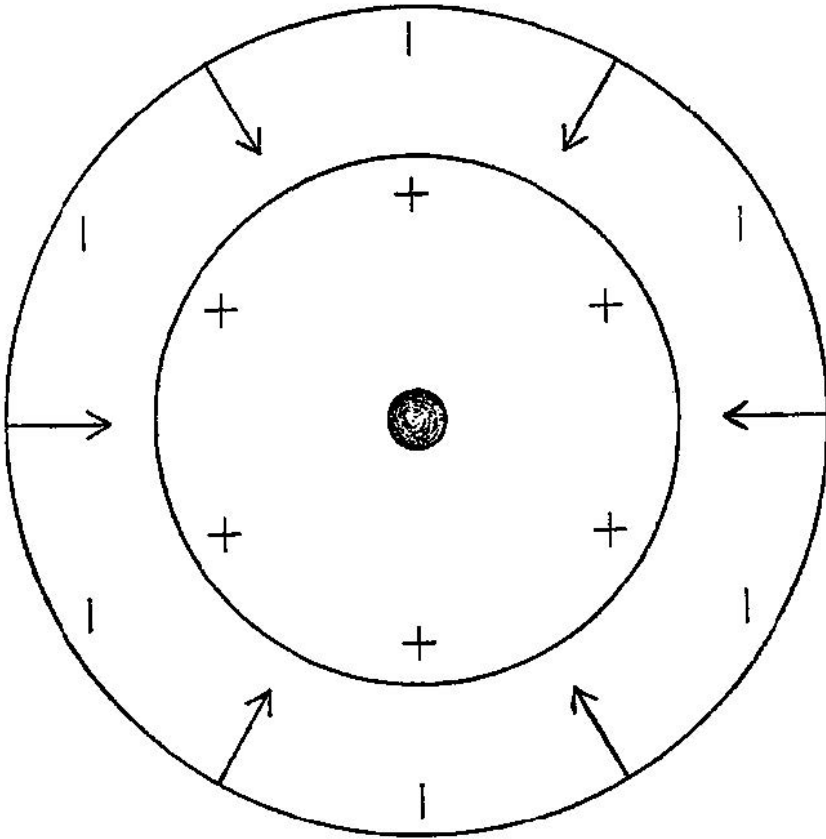


Fig. 2. A cross section of the cylinder. The inner rigid layer is covered with positive charges and the outer flexible layer, which is covered with negative charges, is seen moving back to its original size. The small black circle denotes the inner wave packets of the moving electron.

In Ref. 2 the authors of the AB effect acknowledge the above mentioned shortcoming and attempt to correct it. They start with a nonseparable wave function (Eq. (19) of Ref. 2) and claim that if certain approximations are introduced then a multiplicative wave function can be applied in the calculation (see page 1518 of Ref. 2). Having this form of the wave function, one finds that a finite shift of the interference pattern is obtained.

Let us examine an alternative calculation where the phase shift is derived from a nonseparable wave function. This wave function is written as follows

$$\Psi = (\Phi_A \psi_A + \Phi_B \psi_B) / \sqrt{2} \quad (3)$$

where ψ denotes the single particle wave function of the moving electron and Φ denotes the wave function of the rest of the system. ψ_A is nonzero only at P_A and ψ_B refers analogously to P_B . For simplicity it is assumed that the charges on the cylindrical layers are not electrons and that no antisymmetrization is required for ψ . It is obvious that this simplification does not affect the results of this work.

The general form of (3) belongs to the nonseparable category. However, it contains, as a special case, the multiplicative form where $\Phi_A = \Phi_B$ during all times. Thus, the application of (3) does not prevent us from obtaining results that are compatible with those of the multiplicative wave function. However, a multiplicative wave function belongs to a subspace of the entire Hilbert space. Thus, its results are limited and one cannot be sure that they will agree with those obtained from a nonseparable wave function.

Henceforth, \vec{r}_i and e_i , respectively denote the coordinates and the charge of the i 'th particle at the device and i runs from 1 to n . Similarly, \vec{r} and $-e$ denote the coordinates and the charge of the moving electron. Thus, the arguments of the wave functions are $\Phi = \Phi(\vec{r}_1, \dots, \vec{r}_n, t)$ and $\psi = \psi(\vec{r}, t)$.

The Hamiltonian takes the following form

$$H = H_C + H_e + V \quad (4)$$

where H_C denotes the part of the Hamiltonian that operates on the charges of the cylindrical layers, H_e denotes the kinetic energy of the moving electron and V denotes the interaction between the moving electron and the charges on the cylindrical layers (see Eq. (11) of Ref. 2).

Let us examine the null experiment where the potential associated with the cylindrical charges vanishes identically. Thus, the last term of (4) can be ignored in this case. Using (3) and (4), one finds that the Schrödinger equation takes the form

$$i\hbar \frac{\partial \Psi}{\partial t} = [(H_C \Phi_A) \psi_A + (H_C \Phi_B) \psi_B + \Phi_A (H_e \psi_A) + \Phi_B (H_e \psi_B)] / \sqrt{2}. \quad (5)$$

The phase difference between $\Phi_A \psi_A$ and $\Phi_B \psi_B$ is derived from the solution of this equation. In this case the cylinder does not interact with the moving electron and $\Phi_A = \Phi_B$. This result shows that the contribution of H_C to the required phase difference vanishes. Therefore, for each point on the screen, one finds a phase difference associated with the motion of the two wave packets*

$$\delta\alpha = -\frac{1}{\hbar} \left[\int \psi_A^* H_e \psi_A d^3r dt - \int \psi_B^* H_e \psi_B d^3r dt \right]. \quad (6)$$

This phase difference should be compared with the one obtained in the experiment where the cylindrical potential varies in time. Using (3) and (4), one finds the Schrödinger equation

$$i\hbar \frac{\partial \Psi}{\partial t} = (H_C + H_e + V) \Psi = [(H_C \Phi_A) \psi_A + (H_C \Phi_B) \psi_B + \Phi_A (H_e \psi_A) + \Phi_B (H_e \psi_B) + V \Phi_A \psi_A + V \Phi_B \psi_B] / \sqrt{2}. \quad (7)$$

Cross terms like $\int \psi_A^ H_e \psi_B d^3r$ are omitted because at least one of the functions vanishes at every point.

The moving electron travels in a field-free region and it is macroscopically far from the rest of the charges. The classical limit holds in these circumstances and each wave packet of the moving electron takes the same trajectory and the same speed as the corresponding one of the null experiment. Therefore, considering the phase difference, one finds that the contribution of the third and the fourth terms of (7) and that of the analogous ones of (5) are identical.

The potential associated with the cylindrical charges is

$$V(\vec{r}) = \sum_{i=1}^n \int \Phi_i^* \frac{e_i}{|\vec{r} - \vec{r}_i|} \Phi_i d^3 r_1 \dots d^3 r_n. \quad (8)$$

Substituting this expression into the last two terms of (7), one finds the phase shift derived from them

$$\begin{aligned} \delta a_v &= \frac{e}{\hbar} \left[\int \psi_A^* V_A(\vec{r}) \psi_A d^3 r dt - \int \psi_B^* V_B(\vec{r}) \psi_B d^3 r dt \right] = \\ &= \frac{e}{\hbar} \left[\int \psi_A^* \left\langle \sum_{i=1}^n \int \Phi_A^* \frac{e_i}{|\vec{r} - \vec{r}_i|} \Phi_A d^3 r_1 \dots d^3 r_n \right\rangle \psi_A d^3 r dt - \right. \\ &\quad \left. - \int \psi_B^* \left\langle \sum_{i=1}^n \int \Phi_B^* \frac{e_i}{|\vec{r} - \vec{r}_i|} \Phi_B d^3 r_1 \dots d^3 r_n \right\rangle \psi_B d^3 r dt \right] = \\ &= \frac{e}{\hbar} \int \psi_A^* \left\langle \sum_{i=1}^n \int \Phi_A^* \frac{e_i}{|\vec{r} - \vec{r}_i|} \Phi_A d^3 r_1 \dots d^3 r_n \right\rangle \psi_A d^3 r dt. \quad (9) \end{aligned}$$

Electrostatics proves that the potential of the cylindrical layers vanishes at the location of the outer subpacket. Hence, due to the validity of the classical limit, the last term on the second expression vanishes and the final expression (9) follows.

Let us turn to the first two terms of (7). They represent the contribution made by the self energy of the cylindrical layers. Again, using electrostatics, one realizes that the outer wave packet of the moving electron does not affect the overall self-energy of the cylindrical layers. On the other hand, the flexible layer moves in the field of the inner subpacket and its overall self energy varies due to this fact. The difference between the cylindrical self energy of Φ_A and that of Φ_B can be equated to the negative value of the energy of its charges in the electric potential of the moving electron. This energy difference is

$$\begin{aligned} \delta \varepsilon &= \sum_{i=1}^n \int \Phi_A^* \left\langle \int \psi_A^* \frac{e e_i}{|\vec{r} - \vec{r}_i|} \psi_A d^3 r \right\rangle \Phi_A d^3 r_1 \dots d^3 r_n - \\ &\quad - \sum_{i=1}^n \int \Phi_B^* \left\langle \int \psi_B^* \frac{e e_i}{|\vec{r} - \vec{r}_i|} \psi_B d^3 r \right\rangle \Phi_B d^3 r_1 \dots d^3 r_n = \\ &= \sum_{i=1}^n \int \Phi_A^* \left\langle \int \psi_A^* \frac{e e_i}{|\vec{r} - \vec{r}_i|} \psi_A d^3 r \right\rangle \Phi_A d^3 r_1 \dots d^3 r_n. \quad (10) \end{aligned}$$

Here, like in (9), the second term of the first expression vanishes. Multiplying this quantity by $-1/\hbar$ and integrating on the time, one finds that the phase difference related to the self-energy of the cylindrical charges precisely cancels the quantity written in (9).

The foregoing discussion yields the required phase difference. It shows that the contribution of the first two terms of (7) precisely balances that of the last two terms of this expression. Moreover, the phase difference derived from the third and the fourth terms equals the quantity (6) obtained in the null experiment. This conclusion shows that if one utilizes the nonseparable wave function (3), then he is able to prove that, in the two experiments, the interference patterns are the same. In other words, the electric version of the *AB* effect does not exist. It follows that in the example discussed in this section the multiplicative wave function employed in Ref. 2 and the nonseparable one used here, yield contradictory results.

4. Concluding remarks

The consequences of the two discussions that contrast utilizations of a multiplicative wave function with those of the nonseparable one, are distinguished in several aspects. The calculation of the ground state of the Be atom shows that the results of the two different approaches differ quantitatively and that the difference is of the order of one percent. On the other hand, applying the two approaches to the electric version of the *AB* effect, one derives conclusions that are mutually contradictory: the multiplicative wave function, that is used in Ref. 2 yields a finite value for the electric *AB* effect whereas the analysis of a nonseparable wave function carried out in the previous section, shows that this effect does not exist.

Another point is the problem of accuracy (or correctness) of the different results. In the case of the ground state of the Be atom we know that the lower calculated ground state of the Hamiltonian is a better approximation to the real value. Moreover, in this case we know the experimental value which can be used in an evaluation of the goodness of the results. These two criteria prove that, in the case of the ground state of the Be atom, the nonseparable wave function yields a better description of Nature.

Let us turn to the electric *AB* effect. It is mentioned above that there is no experimental test of this effect^{6,7)}. However, it has already been shown that its original derivation²⁾ is unacceptable because it violates the law of energy conservation⁷⁾. This argument indicates that the conclusion of the previous section, which is based upon a wave function embedded in the entire Hilbert space, is valid.

The two examples discussed in this work prove that the nonseparable form of a wave function of a quantum mechanical system of several particles that have interacted in the past, is correct. The example of the ground state of the Be atom shows that, in this case, the multiplicative form of the wave function can be used as a practical approximation. This statement relies upon the fact that the two results differ by less than one percent. On the other hand, the analysis carried out for the electric *AB* effect proves that the two approaches are associated with contradictory conclusions and that the use of a multiplicative wave function yields results that are incompatible with basic laws of physics. Using the results of the

nonseparable wave function, one realizes that the electric version of the AB effect does not exist.

These conclusions indicate a general rule saying that adequate precautions must be taken when a multiplicative wave function is adopted as an approximation.

References

- 1) Y. Aharonov and D. Bohm, *Phys. Rev.* **115** (1959) 485;
- 2) Y. Aharonov and D. Bohm, *Phys. Rev.* **123** (1961) 1511;
- 3) S. N. Ruijsenaars, *Ann. Phys. (NY)*, **146** (1983) 1 and references therein;
- 4) S. M. Roy, *Phys. Rev. Lett.* **44** (1980) 111;
- 5) P. Bocchieri and A. Loinger, *Nuovo Cimento* **47A** (1978) 475;
P. Bocchieri, A. Loniger and G. Siragusa, *Nuovo Cimento*, **51A** (1979) 1;
- 6) P. Bocchieri and A. Loinger, *Lett. Nuovo Cimento* **35** (1982) 469;
- 7) E. Comay, *Phys. Lett.*, **A120** (1987) 196;
- 8) S. Fraga, J. Karwowski and K. M. S. Saxena, *Handbook of Atomic Data*, Elsevier, Amsterdam 1979;
- 9) C. F. Bunge, *Phys. Rev.* **A14** (1976) 1965.

POS LJEDICE NESEPARABILNOSTI KVANTNO-MEHANIČKIH VALNIH FUNKCIJA

ELIAHU COMAY

Raymond and Beverly Sackler Faculty of Exact Sciences, School of Physics and Astronomy, Tel Aviv University, Tel Aviv 61170, Israel

UDK 530. 192

Originalni znanstveni rad

Analiza bazirana na fundamentalnim svojstvima kvantne mehanike pokazuje da ne postoji električni Aharonov-Bohm efekt. Takav zaključak nije inkompatibilan s eksperimentom. Diskutirano je značenje neseeparabilne prirode kvantno-mehaničkih valnih funkcija.