METHODOLOGICAL NOTES

The exclusion principle and indistinguishability of identical particles in quantum mechanics

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The connection between the exclusion principle and the principle of indistinguishability of identical particles in quantum mechanics is discussed. It is shown with the aid of a density matrix defined for states with arbitrary permutation symmetry that the particles are indistinguishable only for one-dimensional representations of the permutation group (symmetrical and antisymmetrycal), and are distinguishable in all the states that are degenerate in the permutations. It is demonstrated by the same token that the exclusion principle follows from the principle of indistinguishability of identical particles and the Pauli theorem on the connection between spin and statistics.

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CONTENTS

"Seek the source of everything,
and you will understand much."
Koz'ma Prutkov

1. INTRODUCTION. THE EXCLUSION PRINCIPLE

Even though Pauli had established his principle even before the creation of quantum mechanics, and the more general exclusion principle immediately after its birth, nevertheless even now, when quantum mechanics has marked its 50th anniversary, there is no meeting of minds when it comes to the question: Is the exclusion principle a postulate that stems from the experimental data, or a consequence of other postulates of quantum mechanics? I shall discuss in this note the existing viewpoints, and in concluding, I shall prove rigorously that the exclusion principle stems from the principle of indistinguishability of identical particles and Pauli's theorem on the relationship between spin and statistics. But let us have a little history to start.

Wolfgang Pauli arrived at formulating his principle in explaining the regularities in the classification of the spectral terms of atoms in a strong magnetic field. In [1], which was submitted for publication in January 1925, Pauli formulated his principle as follows:

"In an atom there cannot be two or more equivalent electrons for which the values of all four quantum numbers coincide. If an electron exists in an atom for which all of these numbers have definite values, then this state is 'occupied'."

For Pauli, the fourth quantum number was not described by any model. He called the property associated with it the "characteristic two-valuedness of the quantum properties of the electron, which cannot be described classically."[2]

Now we call this two-valued nature of the electron that is not amenable to classical description the spin. In anticipating the quantum nature of the magnetic moment of the electron before the creation of quantum mechanics, Pauli exhibited striking intuition. Interestingly, this same intuition together with Pauli's inherent rigor of thought did not allow him immediately to acknowledge the spin hypothesis that had been advanced by Kronig and independently by Uhlenbeck and Goudsmit to explain the source of the fourth quantum number of the electron. Pauli's objections involved the fact that this hypothesis was based on the classical concept of rotation of the electron about its own axis. And even though Uhlenbeck and Goudsmit[3] explained the doublet splitting in the spectra of the alkali metals by assuming that the ratio of the intrinsic magnetic moment of the rotating electron to the mechanical moment was twice as great as in orbital motion, Pauli was very skeptically inclined toward their hypothesis. Upon meeting Bohr, who had fallen under the influence of explaining the doublet splitting by favoring the rotating-electron hypothesis, Pauli expressed the regret that a new "heresy" had arisen in atomic physics.[4]

Now we know that Pauli was right in not agreeing with the classical interpretation of the fourth degree of freedom. The spin cannot in principle be described by a classical model. In his Nobel lecture, Pauli recalls:[5]

". . . Although at first I strongly doubted the correctness of this idea because of its classical mechanical character, I was finally converted to it by Thomas'[6] calculations on the magnitude of doublet splitting. On the other hand, my earlier doubts as well as the cautious expression 'classically non-describable two-valuedness' experienced a certain verification during later developments, as Bohr was able to show on the basis of wave mechanics that the electron spin cannot be measured by classically describable experiments (as, for instance, deflection of molecular beams in ex-

ternal electromagnetic fields) and must therefore be considered as an essentially quantum mechanical property of the electron."

The first studies devoted to applying the newborn quantum mechanics to many-particle systems were those of Heisenberg[7] and Dirac.[8] These studies derived the principle that Pauli had formulated, that two electrons are forbidden to exist in the same quantum state, as a consequence of the antisymmetry of the wave function of the system of electrons. Dirac[8] came to the conclusion here that light quanta must be described by symmetric wave functions. He especially noted that a system of electrons cannot be described by symmetric wave functions, since the latter allow any number of electrons to exist in a single quantum state.

Thus, with the creation of quantum mechanics, the prohibition on the occupation number of states of a system of electrons was replaced by the more general prohibition of all types of permutational symmetry of wave functions except for antisymmetry. Analysis of experimental data later permitted formulation of an exclusion principle for all known particles, rather than electrons alone. Namely: the only states of a system of identical particles of spin s that are realized are those whose total wave function is multiplied by $(-1)^{2s}$ upon interchange of any pair of particles. That is, it is symmetric for integer values of s (Bose-Einstein statistics) and antisymmetric for half-integer s (Fermi-Dirac statistics).

The exclusion principle also holds for the permutational symmetry of the constituent particles, e.g., of nuclei. Depending on the value of the spin of the nuclei, one can speak of boson nuclei and fermion nuclei. Moreover, if an arbitrary system of particles can be represented as a set of identical subsystems, the symmetry of the wave function of the system with respect to permutations of the subsystems is determined by the value of the total spin of the latter. This permits one to classify subsystems into boson and fermion types. This approach has proved to be very convenient in finding the allowed states of complicated many-atom systems.[9]

In the formulation given above, the exclusion principle leads to an entire series of physically important consequences. One of them is the effective repulsion between constituent particles that consist of identical fermions.[10-11] Repulsion arises at interparticle distances at which the overlap of their wave functions becomes appreciable, and it is entirely due to the requirement of antisymmetry of the wave functions of the system with respect to interchange of fermions between the particles.

Another well-known example consists in molecules having identical nuclei. Let us consider the $^{16}O_2$ molecule. The ^{16}O oxygen nuclei consist of an even number of fermions, and hence they are bosons. Moreover, the nuclear spin s = 0. This inplies that the total wave function of the $^{16}O_2$ molecule, which coincides in this case with the coordinate wave function (since s = 0), must be symmetric with respect to interchange of the nuclei. In the ground electron-vibrational state, this leads to forbidding all rotational levels having odd values of the rotational moment.

The exclusion principle is a generalization of the experimental data. This fact never satisfied Pauli. In his Nobel lecture[5] which he read in 1946, he said:

"Already in my original paper I stressed the circumstance that I was unable to give a logical reason for the exclusion principle or to deduce it from more general assumptions. I had always the feeling, and I still have it today (my underlining–I.K.), that this is a deficiency."

Pauli[12] made a substantial step forward in creating a basis for the exclusion principle in 1940 in his famous theorem of the relation of the spin to statistics. In this theorem, Pauli showed that the field operators of particles with integral spin cannot obey the fermion commutation relationships, since this leads to violation of the causality principle. The field operators of particles of half-integral spin cannot obey the boson commutation relationships, since this leads to negative values of the total energy of the system. Hence he concluded that particles of integral spin obey the Bose-Einstein statistics, while particles of half-integral spin obey the Fermi-Dirac statistics.

This proof, just like the subsequent ones,[13,14] implicitly postulates that only two types of commutation relationships are possible for the field operators: boson and fermion. Yet Green[15] and independently Volkov[16] had shown that field operators that satisfy the principle of causality, relativistic invariance, and positive energy can obey commutation relationships that are more general than boson and fermion types. These are the so-called paraboson and parafermion commutation relationships. The parastatistics corresponding to them is characterized by p-fold occupancy of the one-particle states. When p = 1, the parastatistics goes over into the Fermi-Dirac statistics, and when $p \to \infty$, into the Bose-Einstein statistics.[17] While bosons and fermions show a one-to-one correspondence between the description of the system in configuration space by symmetric and antisymmetric wave functions and the commutation relationships for the field operators, this is no longer the case for the parastatistics. One cannot establish a one-to-one connection between the form of the permutational relationships for the parafield operators and the permutational symmetry of the wave function in configuration space.[18] This implies that the Pauli theorem leaves open the problem of the relation between the spin value and the permutation symmetry of the wave function, independently of whether parastatistics is realized.[1)]

In order to show that the exclusion principle rigorously follows from the Pauli theorem, we must prove that a system of identical particles can be described by only two types of wave functions: symmetric and antisymmetric. This does not follow from the Schrödinger equations, since solutions having arbitrary permutational symmetry satisfy it. The next section is concerned with discussing the situation that arises in this regard and with analyzing critically the existing viewpoints.

[1)]No particles obeying parastatistics have been discovered among the currently known elementary paricles. As Chernikov [19] has shown (see also [20,21]), ordinary fermions that differ in internal quantum numbers obey parafermion commutation relationships. Thus, the nucleons in the nucleus (n, p) can be described by a para-Fermi statistics with a maximum occupation number p=2, and the triplet of quarks (Q_n, Q_p, Q_λ) by a para-Fermi statistics with p=3 [21,22]. One can show that quasiparticles in a periodic lattice (Frenkel excitons, magnons) obey a para-Fermi statistics.

2. THE PRINCIPLE OF INDISTINGUISHABILITY OF IDENTICAL PARTICLES AND THE SYMMETRY POSTULATE

By its very definition of identity, the Hamiltonian of a system of identical particles is invariant with respect to permutation of the particles. Consequently, the Schrödinger equation of a system of N identical particles is satisfied by any linear combination of solutions that differ by permutations of the coordinates of the particles. As we know from the theory of permutation groups, these linear combinations can be classified in terms of symmetry type into different sets that do not mix with one another in the permutations. In other words, they form bases for the irreducible representations of the permutation groups. It is pertinent here to recall to the reader that every irreducible representation of a permutation group can be correlated with some division of the number N into integral positive terms $\lambda^{(i)}$ ($\Sigma\,\lambda^{(i)} = N$), as can be depicted graphically in the form of the so-called Young pattern.[23-24] Young patterns are customarily denoted by the symbol $[\lambda] \equiv [\lambda^{(1)} \ldots \lambda^{(m)}]$, where $\lambda^{(i)}$ is the number of cells in the ith row; the existence of rows having the same number of cells is denoted by the order of the corresponding $\lambda^{(i)}$. The Young patterns characterize the symmetry type of the basis functions with respect to permutation of the arguments. A Young pattern of one row $[N]$ corresponds to a symmetric function, while a Young pattern of one column $[1^N]$ corresponds to an antisymmetric function (the irreducible representations $\Gamma[N]$ and $\Gamma[1^N]$ are one-dimensional). All the other Young patterns $[\lambda]$ correspond to intermediate symmetry types. The irreducible representations $\Gamma[\lambda]$ that they characterize are always multidimensional. That is, they describe states that are degenerate with respect to permutations.

According to the exclusion principle, a system of identical particles can only exist in states that are nondegenerate with respect to permutations: symmetric and antisymmetric. All other symmetry types are forbidden. It is a valid question whether this restriction on the solution of the Schrödinger equation stems from the fundamental principles of quantum mechanics, or is an independent principle.

A number of investigators,[25-28] including one of the founders of quantum mechanics, Dirac, believe that there are no fundamental rules forbidding the existence in nature of particles described by wave functions having more complex permutational properties than those of the fermions and bosons, while the existing restrictions arise only from the properties of the particles known to us. Messiah even introduced the term: the symmetry postulate, thus emphasizing the primary nature of the restrictions on the allowed types of permutational symmetry of the wave function. Upon applying Schur's lemma, Messiah and Greenberg[28] showed that the existence of a permutational expression should introduce no additional uncertainty into the characteristics of a state. The latter result is also directly implied by the Wigner-Eckart theorem in the form in which Koster cast it.[24,29] The matrix element of any operator $\hat{L}$ that is symmetric with respect to all particles, according to Eq. (4.40) in [24], is equal to

$$\langle \Psi_r^{[\lambda]} | \hat{L} | \Psi_{\bar{r}}^{[\lambda]} \rangle = \delta_{r\bar{r}} \langle [\lambda] \| \hat{L} \| [\lambda] \rangle, \qquad (1)$$

Here the subscript r gives the order numbers of the basis functions of the representation of the permutation group $\Gamma[\lambda]$. The double line in the matrix element on the right-hand side of (1) indicates independence of the subscripts r and $\bar{r}$. Thus, the mean value of the operator $\hat{L}$ is the same for all of the functions $\Psi[\lambda]_r$ that belong to the degenerate state.

On the other hand, a number of textbooks and monographs[23,30-32] derive the exclusive realization of states that are nondegenerate with respect to permutations from the principle of indistinguishability of particles in quantum mechanics. However, as is correctly noted in [28], the usually supplied proofs contain additional conditions that do not stem from anything. Thus, the following proof is typical.

From the requirement that the states of a system which one gets by permuting identical particles are physically completely equivalent, the conclusion is drawn that the wave function must vary only by an inconsequential phase multiplier upon transposition of two particles:

$$\Psi(x_2, x_1) = e^{i\alpha} \Psi(x_1, x_2). \qquad (2)$$

Here α is a real constant, and x is the set of spatial and spin variables. The subsequent action of the permutation $\hat{P}_{12}$ on (2) gives

$$\Psi(x_1, x_2) = e^{i2\alpha} \Psi(x_1, x_2), \qquad (3)$$

or

$$e^{2i\alpha} = 1, \quad e^{i\alpha} = \pm 1. \qquad (4)$$

Since all the particles are assumed to be identical, the wave function must behave exactly in the same way with respect to interchange of any pair. That is, it should be either fully antisymmetric or symmetric.

The given proof associates the indistinguishability of identical particles directly with the behavior of the wave function. Moreover, since the wave function is not an observable, the indistinguishability principle is associated with it only indirectly via the expressions for observable quantities. The widespread opinion is false that wave functions that describe the same particular physical state can differ only by a phase coefficient. Thus, according to (1), the values of the physical quantities that characterize a system of identical particles are the same for all functions that belong to a single irreducible representation of the permutation group. Hence all these functions describe a single physical state. The requirement that the function can vary only by a phase coefficient upon permutation is actually to postulate that the representation is one-dimensional. If only the one-dimensional representations ($[\lambda] = [2], [1^2]$) are realized for two particles, then for $N > 2$, all of the representations except $[\lambda] = [N], [1^N]$ are multidimensional, and we must still prove that a wave function that transforms in permutations into a linear combination of functions that belong to a given degenerate state is incompatible with the principle of indistinguishability.

One can rigorously carry out such a proof, but here one must start with a correct formulation of the principle of indistinguishability of identical particles. One of these formulations is the following:

All observable quantities are invariant with respect to the operation of interchange of identical particles, and conversely, interchanges of identical particles cannot be observable.

Since physical quantities are expressed in the matrix formulation of quantum mechanics as bilinear forms of the wave functions, the indistinguishability principle requires the invariance of these bilinear forms:

$$\hat{P}\,\langle\Psi\mid\hat{L}\mid\Psi\rangle=\langle\Psi\mid\hat{L}\mid\Psi\rangle. \tag{5}$$

Since the operators $\hat{P}$ are unitary, Eq. (5) implies that the following commutator is zero:[28]

$$[\hat{P}\hat{L}]=0. \tag{6}$$

Often one restricts the treatment to requiring that the probability of a given configuration of a system of identical particles be invariant with respect to permutations:[33-35]

$$\hat{P}\mid\Psi(x_1,\ldots,x_N)\mid^2\equiv\mid\hat{P}\Psi(x_1,\ldots,x_N)\mid^2=\mid\Psi(x_1,\ldots,x_N)\mid^2. \tag{7}$$

Evidently, (7) is a special case of (5). In order that a function should satisfy (7), it suffices that permutations should transform it as

$$\hat{P}\Psi(x_1,\ldots,x_N)=e^{i\alpha_P(x_1,\ldots,x_N)}\Psi(x_1,\ldots,x_N), \tag{8}$$

That is, in contrast to the requirement (2), the phase in the general case is a function of the coordinates and of the permutation. Evidently, the equations (3) and (4) are not satisfied here.

By adducing the topological properties of configuration space, Girardeau[34] has proved that functions that satisfy the indistinguishability principle in the form of (7) are transformed according to one of the one-dimensional representations of the permutation group at all points of configuration space. Preliminary proofs with a series of restrictions have been given in [33,35]. (For a critique of the proofs of the symmetry postulate that are found in the earlier studies, see [28,33].)

Salzmann[36] has proposed another approach to proving the symmetry postulate. It is based on the assertion that the result of permutations is unobservable, and therefore, a permutation operator cannot be used to distinguish the wavefunctions that belong to a given energy level. Hence the mean value of the permutation operator must be the same for all functions. And the latter is fulfilled only for one-dimensional representations. We cannot grant that this proof is convincing. The possibility of identifying the wavefunctions in terms of the eigenvalues of a permutation operator need not lead actually to distinguishing the states. When degeneracy exists with respect to permutations, the mean value of physical operators is the same according to (1) for all basis functions, although the diagonal matrix elements of the operators differ.

The traditional formulation of the indistinguishability principle is the requirement of invariance of observable quantities with respect to permutations of identical particles (Eqs. (5)–(8)). However, one can approach this from the standpoint of indistinguishability of properties of differing particles. These properties can naturally be described by using a one-particle density matrix. A density matrix that is defined for states having arbitrary permutational symmetry is used below in order to formulate the indistinguishability principle directly with respect to the properties of the identical particles themselves, without involving their permutations. This has made possible a direct proof of the distinguishability of particles in all permutational states except for nondegenerate ones, i.e., except for symmetric and antisymmetric ones.

Thus, our results as well as those of Girardeau[34] inply that the restrictions on the permutational symmetry of the solutions of Schrödinger's equation stem from the indistinguishability principle. This conclusion, together with that of Pauli's theorem that particles of integral spin cannot be described by antisymmetric wavefunctions, while particles with half-integral spin cannot be described by symmetric functions, fully proves the exclusion principle.

3. FORMULATION OF THE INDISTINGUISHABILITY PRINCIPLE IN TERMS OF THE DENSITY MATRIX AND PROOF OF THE SYMMETRY POSTULATE

Let us introduce the one-particle density matrix for a system of N particles in a state having a permutational symmetry characterized by some standard Young pattern $[\lambda]$ consisting of N cells. In line with the fact that the wavefunctions that describe such states belong to an f_λ-dimensional representation $\Gamma^{[\lambda]}$ of the permutation group π_N, the density matrix is characterized by two further indices in addition to the index of the representation $[\lambda]$: the index r of the column of the representation with respect to which the given wavefunction is transformed, and the index t that distinguishes the equivalent irreducible representations

$$\rho_{rt}^{[\lambda]}(x_i',x_i)=\int\Psi_{rt}^{[\lambda]}(x_1,\ldots,x_i',\ldots,x_N)^*\,\Psi_{rt}^{[\lambda]}(x_1,\ldots,x_i,\ldots,x_N)\,dV^{(i)}; \tag{9}$$

Here $dV^{(i)}$ denotes a volume element of the configuration space of the system lacking the i-th particle; in order to abbreviate the notation, the summation over the discrete spin variables is included in the integral sign.

The mean value of the one-particle operator $\hat{f}(\mathbf{x}_i)$ that characterizes some property of the i-th particle of the system[2] in a state having the wave function of the system $\Psi^{[\lambda]}_{rt}$ is defined as

$$\bar{f}_i=\int\hat{f}(x_i)\,\rho_{rt}^{[\lambda]}(x_i',x_i)\big|_{x_i'=x_i}\,dx_i. \tag{10}$$

If particles are to be indistinguishable, the condition must be satisfied that

$$\bar{f}_i=\bar{f}_j=\bar{f}\quad\text{for all i, j.} \tag{11}$$

That is, the quantity (10) must depend on the order number of the particle. A dependence of (10) on the order number of the particle implies that the particles are not equivalent in the state being studied, and hence, they are distinguishable. We shall treat Eqs. (10) and (11) as being a mathematical formulation of the indistinguishability principle.

Let us restrict the treatment to nonrelativistic systems that exist in steady states. We can easily show that it suffices here to study a system of noninteracting particles. The wave vector $|\Psi\rangle$ of a system of interacting nonrelativistic particles that is characterized by the Hamiltonian

$$\hat{\mathcal{H}}=\hat{\mathcal{H}}_0+V, \tag{12}$$

is defined in the same Hilbert space as the wave vector

[2]Such a directly observable property might be, e. g., the probability that the i-th particle will be removed from a bound state of N particles by an external action on the system. Thus, the probability of photoionization in the nonrelativistic theory is determined by the value of the matrix element of the operator $f_i=(\mathbf{e}\cdot\mathbf{p}_i)\,e^{i\mathbf{k}\cdot\mathbf{r}_i}$, where e and k are the polarization vector and the wave vector of the photon, and $\mathbf{p}_i$ and $\mathbf{r}_i$ are the momentum operator and the radius vector of the i-th particle.

$|\Psi_0\rangle$ of the system lacking interaction, and it can be derived from the latter by using some unitary transformation

$$|\Psi\rangle = \hat{U}\,|\Psi_0\rangle. \tag{13}$$

In order to find the form of this unitary transformation, we can use the well-known relationship that the series of the Brillouin-Wigner[37] permutation theory is based on:

$$|\Psi\rangle = |\Psi_0\rangle + \frac{\hat{Q}}{E-\hat{\mathcal{H}}_0}\hat{V}|\Psi\rangle. \tag{14}$$

Here $\hat{Q}$ is the projection operator that projects an arbitrary vector onto the multitude of vectors of Hilbert space that are orthogonal to the vector $|\Psi_0\rangle$. Upon substituting Eq. (13) into (14), we get an equation for $\hat{U}$, from which we find

$$U^{-1} = 1 - \frac{\hat{Q}}{E-\hat{\mathcal{H}}_0}\hat{V}. \tag{15}$$

Since the interaction operator $\hat{V}$ of the identical particles, just like $\hat{\mathcal{H}}_0$, is invariant with respect to permutations of identical particles, the operator $\hat{U}$ is also invariant. Hence, according to (13), the permutational symmetry of the states $|\Psi\rangle$ and $|\Psi_0\rangle$ coincides.

Let us treat a system of N noninteracting identical particles. Each particle is characterized by an orthonormal set of one-particle functions $\{\Psi_a\}$. The state of the entire system is characterized by assigning a certain configuration of the one-particle states

$$K:\quad \psi_a^{n_a}\psi_b^{n_b}\ldots\psi_q^{n_q},\quad \sum_c n_c = N, \tag{16}$$

$$n_a \geqslant n_b \geqslant \ldots \geqslant n_q \tag{17}$$

and the permutational symmetry of some Young pattern $[\lambda]$ consisting of N cells. We shall impose no restrictions on the values of the occupation numbers n_c in (16). The ordering in (17) is convenient for characterizing the state with a standard Young pattern whose row length satisfies the condition

$$\lambda^{(1)} \geqslant n_a, \quad \lambda^{(2)} \geqslant n_b, \ \ldots$$

We shall construct the wave functions of the system that belong to the basis of an irreproducible representation $\Gamma^{[\lambda]}$ of the permutation group from products of the one-particle functions

$$\Psi_0(K) = \psi_a(x_1)\ldots\psi_a(x_{n_a})\,\psi_b(x_{n_a+1})\ldots\psi_q(N) \tag{18}$$

by using the Young operators $\omega^{[\lambda]}_{rt}$ (see Eq. (2.30) in [24]):

$$\Psi^{[\lambda]}_{rt}(K) = \omega^{[\lambda]}_{rt}\Psi_0(K) = N^{[\lambda]}(K)\sum_{\hat{P}}\Gamma^{[\lambda]}_{rt}(\hat{P})\,\hat{P}\Psi_0(K). \tag{19}$$

The subscript r gives the order number of the f_λ basis functions of the representation $\Gamma^{[\lambda]}$, and the subscript t gives the order number of the independent bases that can be constructed from the functions $\hat{P}\Psi_0(K)$. In line with the fact that the one-particle functions in (18) include some coincident ones, the normalizing factor is

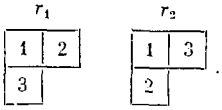
$$N^{[\lambda]}(K) = \sqrt{\frac{f_\lambda}{n_a!\ldots n_q!\,N!}}. \tag{20}$$

Before we study the expression for the mean value of the one-particle operator (10) in the general case of a system of N identical particles, let us study a system of three particles for the sake of its graphic quality. Here we can easily write out the explicit form of the functions that belong to the irreproducible representations of the permutation group of three objects, and calculate "in our heads" the mean value of the one-particle operator.

Let us study a configuration of the one-particle states: $\psi_a^2\psi_b$. We can construct for such a configuration one totally symmetric function

$$\Psi^{[3]} = \frac{1}{\sqrt{3}}\left[\psi_a(1)\psi_a(2)\psi_b(3) + \psi_a(1)\psi_a(3)\psi_b(2) + \psi_a(3)\psi_a(2)\psi_b(1)\right] \tag{21}$$

and two functions that transform according to a two-dimensional irreducible representation $\Gamma^{[\lambda]}$ that are characterized by the Young patterns



We can easily find the form of the functions by using the Young operators $\omega_{11}^{[21]}$ and $\omega_{21}^{[21]}$ (see Eq. (2.39) in [24]) (only one basis of the representation $\Gamma^{[21]}$ can be constructed for the configuration $\psi_a^2\psi_b$, and hence the subscript t that normalizes the bases is not needed):

$$\Psi_1^{[21]} = \frac{1}{\sqrt{6}}\left\{2\psi_a(1)\psi_a(2)\psi_b(3) - \psi_a(1)\psi_a(3)\psi_b(2) - \psi_a(3)\psi_a(2)\psi_b(1)\right\}.$$

$$\Psi_2^{[21]} = \frac{1}{\sqrt{2}}\left\{\psi_a(1)\psi_a(3)\psi_b(2) - \psi_a(3)\psi_a(2)\psi_b(1)\right\}. \tag{22}$$

Direct calculation shows that if the following expression holds for the function $\Psi^{[3]}$:

$$\langle\Psi^{[3]}|\hat{f}_i|\Psi^{[3]}\rangle = \frac{1}{3}(2f_{aa} + f_{bb}) \quad \text{for } i = 1, 2, 3,$$

where f_{aa} denotes $\langle\psi_a(i)|\hat{f}_i|\psi_a(i)\rangle$, then for the function of (22),

$$\left.\begin{aligned}
&\langle\Psi_1^{[21]}|f_i|\Psi_1^{[21]}\rangle = \tfrac{1}{6}(5f_{aa} + f_{bb}) \quad \text{for } i = 1, 2,\\
&\langle\Psi_1^{[21]}|f_3|\Psi_1^{[21]}\rangle = \tfrac{1}{3}(f_{aa} + 2f_{bb}),\\
&\langle\Psi_2^{[21]}|f_i|\Psi_2^{[21]}\rangle = \tfrac{1}{2}(f_{aa} + f_{bb}) \quad \text{for } i = 1, 2,\\
&\langle\Psi_2^{[21]}|f_3|\Psi_2^{[21]}\rangle = f_{aa}.
\end{aligned}\right\} \tag{23}$$

The matrix elements for the third particle differ from the corresponding ones for the first two particles. Hence, the indistinguishability criterion is not fulfilled for states that are described by wave functions belonging to the two-dimensional representation $\Gamma^{[21]}$. The coincidence of the matrix elements for the first two particles involves the fact that the function $\Psi_1^{[21]}$ is symmetric with respect to them, while $\Psi_2^{[21]}$ is antisymmetric.

Now let us examine an arbitrary state of a system of N particles having the configuration of (16), as characterized by the wave function of (19). Let us substitute the expression for $\Psi^{[\lambda]}_{rt}(K)$ into the definition of the density matrix in (9):

$$\rho^{[\lambda]}_{rt}(x_i', x_i) = N^{[\lambda]}(K)^2\sum_{\hat{P}\hat{\bar{P}}}\Gamma^{[\lambda]}_{rt}(\hat{P})^*\,\Gamma^{[\lambda]}_{rt}(\hat{\bar{P}})$$
$$\times\int\hat{P}\Psi_0(x_1,\ldots,x_i',\ldots,x_N)^*\,\hat{\bar{P}}\Psi_0(x_1,\ldots,x_i,\ldots,x_N)\,dV^{(i)}. \tag{24}$$

The permutations $\hat{P}$ can always be represented as products $\hat{P}'\hat{P}_{ic}$, where the $\hat{P}_{ic}$ bring the particle i to the site of a particle existing in the state ψ_c, while $\hat{P}'$ does not act on the particle i. That is, $\hat{P}'$ belongs to the permutation group π_{N-1} that is obtained from π_N by removing the i-th particle. This permits us to remove $\psi_c(x_i)$ from inside the integral in (24). If the function ψ_c is contained several times in the configuration (16), then the transfer of the i-th particle to the site of the

arguments by a series of standing functions ψ_c is carried out by the permutation $\hat{P}_{ii_c+1}$, which is related to $\hat{P}_{ii_c}$ by

$$\hat{P}_{ii_c\pm1}=\hat{P}_{i_ci_c\pm1}\hat{P}_{ii_c}\hat{P}_{i_ci_c\pm1}.$$

Since the order numbers of the arguments in the repeated one-particle functions lie in a single row of the Young pattern, the properties of the standard representation of the permutation group imply that (cf. [38]):

$$\Gamma^{[\lambda]}_{rt}(\hat{P}'\hat{P}_{ii_c\pm1})=\Gamma^{[\lambda]}_{rt}(\hat{P}'\hat{P}_{ii_c}). \tag{25}$$

Let us rewrite (24) by replacing the summation over $\hat{P}$ by summation over $\hat{P}'$ and c and taking (25) into account:

$$\rho^{[\lambda]}_{rt}(x_i',\ x_i)=N^{[\lambda]}(K)^2\sum_{\hat{P}'}\sum_{\bar{\hat{P}}'}\sum_{c}\sum_{\bar{c}}n_cn_{\bar{c}}\Gamma^{[\lambda]}_{rt}(\hat{P}'\hat{P}_{ii_c})^*\times\Gamma^{[\lambda]}_{rt}(\bar{\hat{P}}'P_{ii_{\bar{c}}})\psi_c(x_i')^*\psi_{\bar{c}}(x_i)\int\hat{P}'\Psi_0(K_c)^*\,\bar{P}'\Psi_0(K_{\bar{c}})\,dV^{(i)}. \tag{26}$$

Here K_c denotes the configuration K lacking the orbital c. Further, let us represent $\hat{P}'$ in the form $\hat{Q}^{(c)}\hat{P}_e$, where $\hat{Q}^{(c)}$ interchanges particles only between different one-particle functions of the configuration K_c, while $\hat{P}_c$ interchanges them between like functions. If we take account of the orthogonality of the one-particle functions and the properties of the standard representation of the permutation group, after some simple transformations we get[3)]

$$\rho^{[\lambda]}_{rt}(x_i',\ x_i)=\sum_c M^{[\lambda]}_{rt,ic}(K)\,\psi_c(x_i')^*\,\psi_c(x_i). \tag{27}$$

where the coefficients are

$$M^{[\lambda]}_{rt,ic}(K)\quad\frac{n_1!n_a!\ldots n_q!}{N!}\sum_{\hat{Q}^{(c)}}|\Gamma^{[\lambda]}_{rt}(\hat{Q}^{(c)}P_{ii_c})|^2. \tag{28}$$

When we substitute the expression (27) for the density matrix into the definition (10), we find

$$\bar{f}_i=\sum_c M^{[\lambda]}_{rt,ic}(K)\,f_{cc}. \tag{29}$$

The coefficients $M^{[\lambda]}_{rt,ic}$ depend on the order number of the particle i. Hence the mean of f will generally differ for different particles. We can easily convince ourselves that a calculation of the coefficients $M^{[\lambda]}_{rt,ic}$ according to Eq. (28) for $[\lambda]=[21]$ and K: $\psi_a^2\psi_b$ gives the same values as those obtained above upon directly calculating the matrix element; see (23).

Thus the particles are distinguishable in the case of an arbitrary irreducible representation. The exceptions are the one-dimensional representations $\Gamma^{[N]}$ and $\Gamma^{[1^N]}$. In this case, for all permutations,

$$|\Gamma^{[\lambda]}_{rt}(\hat{Q}^{(c)}P_{ii_c})|^2=1$$

and

$$M^{[N],[1^N]}_{rt,\,ic}=\frac{n_c}{N}.$$

We find for $\bar{f}_i$,

$$\bar{f}_i=\frac{1}{N}\sum_c n_cf_{cc}=\bar{f}, \tag{30}$$

That is, the particles are indistinguishable.

[3)]In the special case of the antisymmetric representation $\Gamma[1^N]$, all of the $n_c=1$, and in the converse case the function of (19) vanishes. As we should expect; Eq. (27) goes over into the well-known expression for the Dirac density matrix [37]:

$$\rho^{[1^N]}(x_i',\ x_i)=\frac{1}{N}\sum_c\psi_c(x_i')^*\psi_c(x_i),$$

as defined in terms of the determinant wave functions.

Thus, in spite of the fact that the mean values of the operators that describe the properties of the entire system coincide according to (1) for all wave functions that belong to a state that is degenerate with respect to permutations, an analysis of the one-particle properties shows that the particles are distinguishable in these degenerate states.

This implies that the particles are also distinguishable in states described by a non-symmetrized wave function. One can always represent such a function in the form of a summation:[23,24]

$$\Psi=\sum_{\lambda,r}\Psi^{[\lambda]}_r. \tag{31}$$

Since the particles are distinguishable for all irreducible representations $\Gamma[\lambda]$ except $\Gamma[N]$ and $\Gamma[1^N]$, then the particles must be distinguishable in a state having the function (31). Only one-dimensional representations are realized for two particles. Yet, evidently, a superposition of the functions $\Psi[2]+\Psi[1^2]$ does not satisfy the indistinguishability principle in the form of (7).

We emphasize that the condition that the wave function should belong to a one-dimensional representation of the permutation group is a necessary but not sufficient condition for indistinguishability of particles. A description of a system of particles that differ in their properties (in charge, magnetic moment, etc.) by symmetric or antisymmetric functions does not make them indistinguishable.[4)] A well-known example is the nucleons in the nucleus. The Hamiltonian that includes only the strong interactions is symmetric with respect to the protons and neutrons (isotopic invariance[23]). We can treat formally the proton and neutron as two states of a single particle, the nucleon, which differ in the value of the projection of the isotopic spin. The wave function of the nucleus must be antisymmetric with respect to permutations of the coordinates of all of the nucleons if we permute also the isotopic coordinate along with the spatial and spin coordinates. However, if we take account of the electromagnetic interactions, then the protons become distinguishable from the neutrons, even though one can construct also in this case a symmetric Hamiltonian[33] that allows antisymmetric functions as solutions.

Identical particles can be considered to be distinguishable when they are localized in spatially remote wells. Formally, when we use symmetrized wave functions, we cannot say exactly in which potential well a given particle lies. However, at great distances between the wells, the exchange effects become negligibly small, and cannot be manifested experimentally in any way. The result of a measurement will not contain interference terms, and in line with the approach of Feynman,[40] we must consider the particles to be distinguishable. This can be illustrated graphically by the example of the behavior of the photoionization cross-section of the H_2 molecule as the nuclei are separated.

An expression for the differential cross-section for photoionization of the H_2 molecule has been derived in [41] by approximating the ground state of the molecule by the Heitler-London function and the wave function of the ejected electron by a plane wave. It can be

[4)]Lyuboshitz and Podgoretskiĭ have treated cases of indistinguishability of non-identical particles [39].

represented in terms of the atomic photoionization cross-section:

$$\frac{d\sigma_{H_2}}{d\Omega} = \frac{Z^{*5}(1-s_{ab})}{1-s_{ab}^2}\{1+\cos(\mathbf{k}-\mathbf{q},\mathbf{R})\}\frac{d\sigma_H}{d\Omega}. \quad (32)$$

Here $\mathbf{k}$ and $\mathbf{q}$ are the wave vectors of the proton and the electron, $|\mathbf{R}|$ is the equilibrium distance between the nuclei, and $s_{ab} = \langle\varphi_a^{is}|\varphi_b^{is}\rangle$ is the overlap integral of the atomic wave functions. $Z^* = 1.19$ is the effective Slater charge, the value of $Z^* \neq 1$ because of perturbation of the atomic electron cloud by the adjacent H atom. The cross-section contains the interference term $1 + \cos(\mathbf{k}-\mathbf{q},\mathbf{R})$ that arises from the equal probabilities of ejection of the electron from the centers a and b.

As the distance between the atoms is increased, their interaction declines, and $Z^* \to 1$, while the overlap integral $s_{ab} \to 0$. In the final state, an electron can be ejected either from atom a or atom b. The expression for the photoionization cross-section as derived with the antisymmetrized functions has a form analogous to (32) with $s_{ab} = 0$:

$$\frac{d\sigma_{2H}^{g,u}}{d\Omega} = (1 \pm \cos(\mathbf{k}-\mathbf{q},\mathbf{R}))\frac{d\sigma_H}{d\Omega}. \quad (33)$$

The upper sign corresponds to a state that is symmetric with respect to the inversion operation, and the lower sign to an antisymmetric state. Both of these states correspond to the same energy for separated atoms, and hence

$$\frac{d\sigma_{2H}}{d\Omega} = \frac{d\sigma_{2H}^{g}}{d\Omega} + \frac{d\sigma_{2H}^{u}}{d\Omega} = 2\frac{d\sigma_H}{d\Omega},$$

That is, the cross section contains no interference terms. The photoionization process occurs independently in each of the atoms. In principle, we can identify the atom from which the electron was ejected.

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