45 (1969); L. J. Kijewski, J. K. Percus, I. H. Pratt,

and J. P. Tranchina, Phys. Rev. A $\underline{2}$, 310 (1970). ³M. Rosina, J. K. Percus, L. J. Kijewski, and G.

Garrod, J. Math. Phys. <u>10</u>, 1761 (1969).

⁴This is equivalent to the G-matrix symmetry condition of C. Garrod and M. Rosina, J. Math. Phys. 10,

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1855 (1969).

⁵See, e.g., M. E. Rose, *Elementary Theory of Angular Momentum* (Wiley, New York, 1957). ⁶P. M. Morse, L. A. Young, and E. S. Haurwitz, Phys. Rev. <u>48</u>, 948 (1935).

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Exchange Symmetry of Many-Particle State Functions*

W.R. Salzman

Department of Chemistry, University of Arizona, Tucson, Arizona 85721 (Received 17 October 1969; revised manuscript received 15 June 1970)

A formal operator definition of indistinguishability of identical particles alternative to permutation invariance of configuration probabilities is presented. The exchange-symmetry properties of many-particle wave functions are shown to follow simply and directly from the new definition.

INTRODUCTION

The requirement that state functions for systems of identical particles be either totally symmetric or totally antisymmetric under interchange of the coordinates¹ of two of the particles is so well established experimentally that it is often presented as a fundamental postulate of quantum mechanics (the symmetrization postulate).²⁻⁴ Upon agreement that particles with totally symmetric states are called bosons and particles with totally antisymmetric states are called fermions, the symmetrization postulate may be stated: *All particles are either fermions or bosons*. States with other symmetries are conceivable but particles have not been found in nature to fit them.

The relatively late introduction of the symmetrization postulate into the logical scheme of quantum mechanics contributes to the feeling that it is an ad hoc assertion introduced at the last minute to make the theory fit experiment. It would be more pleasing to derive the symmetrization postulate from general principles and the indistinguishability of identical particles. Accordingly, a number of workers have attempted to reduce the symmetrization postulate to a theorem, 5-11 but most attempts so far have either been based on assumptions which are not generally true or have placed seemingly unnecessary restrictions on the type of physical systems to which they apply. Girardeau,⁹ after pointing out the deficiencies of previous arguments, presented a proof of the symmetrization postulate which depends in an essential way on the topology of the configuration space of the particles (in particular the argument depends on the connectedness of the configuration space). Since there exists an

interesting class of systems¹² for which the topological requirements do not hold, the proof seemed to be unnecessarily restricted. The connectedness restriction on configuration space was lifted by Flicker and Leff¹⁰ for the case of particles with no internal degrees of freedom, and then for the general case by Giradeau.¹¹ These more recent proofs are still topological in nature and use the permutation invariance of configurational probabilities (stated variously as $|\underline{P\Psi}|^2 = |\Psi|^2$ or $\underline{P}|\Psi|^2 = |\Psi|^2$ for every Ψ) as the fundamental definition of particle indistinguishability. They thus are very strongly tied to a particular representation of quantum mechanics, namely, the configuration-space representation.

In the present paper we offer an alternative definition of particle indistinguishability which, although more formal and lacking the lucid pictorialization of permutation invariance, characterizes the indistinguishability of identical particles realistically. In particular, we show that the statement "the exchange of two identical (indistinguishable) particles is not observable" leads directly and unambiguously to the result "identical particles are either fermions or bosons." The first statement implicitly defines identical particles as those whose interchange is not observable.

We first establish that this definition is reasonable and has precedent and then show that it leads directly and simply to the desired result.

PERMUTATIONS OF INDISTINGUISHABLE PARTICLES

The set of N! operations which produce all possible permutations of the coordinates of N particles form the group S_N , the symmetric group of order

N.¹³ The Hilbert space for N identical particles¹⁴ may be unambiguously factored into orthogonal irreducible subspaces corresponding to irreducible representations of S_N .¹⁵ Since all of the operators of S_N commute with the Hamiltonian of a system of N indistinguishable particles¹⁶ (and indeed with the operators of all the dynamical quantities definable for the system), it follows that none of the operators representing dynamical quantities can rotate states from one irreducible subspaces form a particularly convenient and natural partitioning of the N-particle Hilbert space; in the following we assume the Hilbert space has been so partitioned.

We restrict our attention to one particular class of operations in S_N , the $\frac{1}{2}N(N-1)$ pair exchange operations (or transpositions) symbolized by $(1^{N-2}, 2)$. A typical member of this class \underline{P}_{ij} exchanges the coordinates of particles *i* and *j*; we shall refer to this class as the exchange class. The entire group S_N can be generated from the exchange class and products of two or more exchange elements (not all products are unique, however). The operators of the exchange class are obviously their own inverse and so have eigenvalues ± 1 , i.e.,

$$\underline{\mathbf{P}}_{ij}^2 = \underline{\mathbf{P}}_{ij} \, \underline{\mathbf{P}}_{ij} = 1, \qquad \underline{\mathbf{P}}_{ij}^{-1} = \underline{\mathbf{P}}_{ij} \, .$$

If $\underline{\mathbf{P}}_{ij} \Psi = a \Psi$ then $a^2 = 1$ and $a = \pm 1$. The operators of the exchange class are Hermitian¹⁷ and linear. (In general, the operators of S_N are linear but not necessarily Hermitian.) Further, we assume that if Ψ is in the *N*-particle Hilbert space so is Ψ' $= \underline{\mathbf{P}}_{ij} \Psi$ (this is clearly true in the usual representations, see Ref. 14), thus the exchange operators are in a formal sense "observables" in quantum mechanics. We shall see shortly that they are "observables" which must be unobservable, and herein lies the crux of the symmetry restrictions for many-particle systems.

OBSERVABLES AND UNOBSERVABLES

In quantum mechanics, linear Hermitian operators whose domain and range are the same Hilbert space are said to represent observables.¹⁸ The nomenclature is reasonable since Hermitian operators have real expectation values and the results of physical measurements are real numbers. However, there is ample precedent¹⁹ for consideration of an aspect of observables other than the generation of real numbers for comparison with experimental results; namely, observables may be used to distinguish between (or label) the various states of a system. That is, if one has a Hermitian operator A, it is possible to distinguish between various states by the values of their expectation values with A, $\langle \Psi | A | \Psi \rangle$.²⁰ (There may be degeneracies, of course, but one can at least use A to distinguish between various sets of states.) It is usually assumed that with a sufficiently large set of Hermitian operators, A, A', A'', \ldots , it is possible to use their expectation values to completely characterize (or label) the states of the Hilbert space. With this second aspect of observables in mind, we can unambiguously define an "unobservable" as a linear Hermitian operator with the same domain as range which cannot differentiate between states of the Hilbert space. If a linear Hermitian operator B is an unobservable then the expectation values $\langle \Psi | B | \Psi \rangle$ must be the same for every state in the Hilbert space; otherwise it would be possible to label (and thus distinguish between) the various states by their expectation value with B.

BOSONS AND FERMIONS

When we say that two particles are identical (or indistinguishable) we really mean that the interchange of the coordinates of the two particles is unobservable. A definition of indistinguishability of identical particles which gives precisely this result is: *Two particles are identical if their interchange is unobservable*. Clearly, one can identify whole sets of identical particles by applying the definition two particles at a time. Thus, for an *N*-identical-particle system the $\frac{1}{2}N(N-1)$ exchange operators \underline{P}_{ij} are unobservables, i.e., they cannot label or distinguish between the various allowable states of the system. If the states Ψ_a , Ψ_b , Ψ_c ,... are in the *N*-particle Hilbert space, we must have

$$\langle \Psi_a | \underline{\mathbf{P}}_{ij} | \Psi_a \rangle = \langle \Psi_b | \underline{\mathbf{P}}_{ij} | \Psi_b \rangle = \cdots$$
 (1)

for all states in the space and for all $\frac{1}{2}N(N-1)$ of the P_{ii} . This statement is not equivalent to the statement that $\underline{\mathbf{P}}_{ij} \Psi = c \Psi$, with c independent of $\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \ldots, \mathbf{x}_N$ (the proof of which statement is the crux of the conventional argument $^{9-11}$). Here the $\langle \Psi_a | \mathbf{P}_{ii} | \Psi_a \rangle$, etc., are expectation values (pure numbers) with any configuration dependence (in the appropriate representation) integrated out. (It is not necessary to assume $\langle \Psi_a | P_{ij} | \Psi_a \rangle$ = $\langle \Psi_a | \mathbf{P}_{jk} | \Psi_a \rangle$, etc.) Clearly only two of the subspaces corresponding to irreducible representations of S_N have the property that all $\frac{1}{2}N(N-1)$ of the P_{ij} 's are unobservable, namely, the totally symmetric and totally antisymmetric subspace. In the totally symmetric subspace all P_{ii} 's are +1 and in the totally antisymmetric subspace all P_{ii} expectation values are -1. The states with intermediate symmetry will be neither totally symmetric nor totally antisymmetric so that there will be at least one of the \underline{P}_{ij} which may be used to label and distinguish between the states of the same irreducible subspace (see Appendix).

Thus, it is a necessary consequence of our definition of indistinguishability that any system having states with intermediate symmetry is necessarily composed of particles which are in some sense distinguishable.

It should be emphasized that the only assumption in the above argument is that all P_{ij} are unobservable; we have not assumed the existence of a complete set of commuting observables nor have we had to make any assumptions about the topology or dimensionality of the configuration space of the particles.

APPENDIX

The statement that states of the same irreducible subspace (with intermediate symmetry) are distinguishable under the P_{ij} operations, i.e., that the P_{ij} are observable in these intermediate subspaces, is readily verified. From any given irreducible subspace we can select a finite set of states which form a basis for the corresponding irreducible representation of S_N . Without loss of generality we can construct from these states an orthonormal, but not complete, set of states. Since the P_{ii} are Hermitian we can find a unitary transformation of our finite orthonormal basis set which brings the matrix representation of a particular one of the \underline{P}_{ij} , say \underline{P}_{12} , to diagonal form. The eigenvalues of \underline{P}_{12} are ± 1 , hence the diagonal elements of this matrix must be ± 1 . The trace of this matrix gives the character of the exchange class for the particular irreducible representation chosen. The rules for constructing the character table for

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¹Coordinates will always refer to *all* coordinates, both internal and external, e.g., position and spin for an electron.

- ²A. M. L. Messiah, *Quantum Mechanics* (North-Holland, Amsterdam, 1961), Vol. II, p. 595.
- ³A. M. L. Messiah and O. W. Greenberg, Phys. Rev. 136, B248 (1964).
- ⁴J. Bros, A. M. L. Messiah, and D. N. Williams, Phys. Rev. 149, 1008 (1966).
 - ⁵J. M. Jauch, Helv. Phys. Acta. <u>33</u>, 711 (1960).
- ⁶J. M. Jauch and B. Misra, Helv. Phys. Acta. <u>34</u>, 699 (1961).
- ⁷D. Pandres, Jr., J. Math. Phys. 3, 305 (1962). ⁸A. Galindo, A. Morales, and R. Nuñez-Lagos, J.
- Math. Phys. 3, 324 (1962).

⁹M. D. Girardeau, Phys. Rev. <u>139</u>, B500 (1965). ¹⁰M. Flicker and H. S. Leff, Phys. Rev. <u>163</u>, 1353 (1967).

- ¹¹M. D. Girardeau, J. Math. Phys. <u>10</u>, 1302 (1969). ¹²M. D. Girardeau, J. Math. Phys. 1, 516 (1960). ¹³A detailed discussion of the symmetric group is given
- in M. Hamermesh, Group Theory and its Application to Physical Problems (Addison-Wesley, Palo Alto, Calif.,

 S_N using Young's tableaux²¹ (which may be rigorously derived) show that for every representation except the totally symmetric (N) and totally antisymmetric (1^N) representations

$$\chi_E > |\chi_{P_{ii}}| ,$$

where χ_E is the character of the identity class (i.e., the dimension of the representation) and $\chi_{P_{ii}}$ is the character of the exchange class. In our diagonal matrix representation of P_{12} , then, some of the diagonal elements are +1 and some are -1, but they are not all the same. Thus, in every subspace except (N) and (1^N) it is possible to use the expectation values of the P_{ii} to distinguish between states of that subspace.

Stated differently, in order for the P_{ij} to be unobservable the matrix representations of the P_{ii} operators in the Hilbert space (which we most assuredly can construct) must be ± 1 , which is only true in subspaces corresponding to the representations (N) or (1^N) of S_N .

Finally we note that linear combinations of symmetric and antisymmetric states are also forbidden since P_{ii} is capable of distinguishing some linear combinations from others. For example, if

 $\Psi_1 = a\Psi_S + b\Psi_A$ and $\Psi_2 = b\Psi_S - a\Psi_A$,

$$\langle \Psi_1 | \underline{\mathbf{P}}_{ij} | \Psi_1 \rangle = a^2 - b^2$$
 and $\langle \Psi_2 | \underline{\mathbf{P}}_{ij} | \Psi_2 \rangle = b^2 - a^2$.

then

¹⁴We have in mind the ordinary nonrelativistic quantum mechanics. For concreteness we will consider the Hilbert space to be the space of all N-particle functions which are square integrable in the variables of every particle (integration includes a summation over discrete variables) since this is the usual space for atomic and molecular problems. This space, as is well known, is spanned by the set of all N-fold products of squareintegrable one-particle functions $\phi_a(x_1) \phi_b(x_2), \ldots,$ $\phi_{e}(x_{N})$. This product realization of Hilbert space is particularly helpful for visualizing the workings of the various permutation operators.

¹⁵Y. Ohnuki and S. Kamefuchi, Ann. Phys. (N. Y.) 51, 337 (1969). ¹⁶Reference 2, p. 594.

¹⁷H. A. Kramers, *Quantum Mechanics* (North-Holland, Amsterdam, 1958), p. 315.

¹⁸Reference 2, Vol. I, p. 298.

¹⁹See, for example, G. C. Wick, A. S. Wightman,

and E. P. Wigner, Phys. Rev. <u>88</u>, 101 (1952). ²⁰One usually sees this stated for representations in

which A is diagonal, but for simply distinguishing between states diagonalization is not necessary.

²¹Reference 13, p. 201.

^{1962),} Chap. 7.