Eigenvalues of Density Matrices*

B. C. Carlson and Joseph M. Keller

Institute for Atomic Research and Department of Physics, Iowa State University, Ames, Iowa

(Received September 8, 1960)

For a system of N identical particles in a pure bound state, the density matrices of positive orders p and $N-p$ have the same nonzero eigenvalues with the same multiplicities. If the number of nonzero eigenvalues is finite, these density matrices are unitarily equivalent.

DENSITY matrices (sometimes specifically called generalized[1] or reduced[2] density matrices) are of interest in describing many-particle systems because many important properties of the system can be calculated from knowledge of a low-order density matrix, without reference to the complete wave function of the system. For example, the energy of a system of particles interacting through two-body forces is completely determined by the second-order density matrix.

The density matrix of order p for a system of N identical particles in a pure state with wave function $\psi(x_1\cdots x_N)$ is defined by

$$\Gamma_p(x_1\cdots x_p; x_1'\cdots x_p')\equiv\binom{N}{p}\int\psi(x_1\cdots x_p,y_{p+1}\cdots y_N)$$

$$\times\psi^*(x_1'\cdots x_p',y_{p+1}\cdots y_N)dy_{p+1}\cdots dy_N. \quad (1)$$

The wave function is assumed to be normalized to unity. The variable x_i stands for the space and spin coordinates of a single particle; the particles may be either fermions or bosons. Letting a single symbol x represent the p variables $x_1\cdots x_p$ and y represent the $N-p$ variables $y_{p+1}\cdots y_N$, we rewrite the definition (1) in the briefer form

$$\Gamma_p(x,x')\equiv\binom{N}{p}\int\psi(x,y)\psi^*(x',y)dy. \quad (1a)$$

A density matrix of order $p>0$ may be regarded as the kernel of a linear integral operator Γ_p in the Hilbert space $\mathfrak{H}_p$ of square integrable functions f of p variables:

$$\Gamma_p f(x)=\int\Gamma_p(x,x')f(x')dx'. \quad (2)$$

We shall now prove that the density operators Γ_p and Γ_{N-p} have the same nonzero eigenvalues with the same multiplicities.

It is easily verified that the scalar product $(f,\Gamma_p f)$ is non-negative for every element f and that the trace of

the density operator is finite:

$$\mathrm{Tr}\Gamma_p=\int dx\,\Gamma_p(x,x)=\binom{N}{p}.$$

Hence the density operator is a non-negative Hermitian operator with finite trace; such an operator has a purely discrete spectrum and its eigenfunctions include a complete orthonormal set.[3] The elements of this set will be denoted by $g_r(x)$ $(r=1, 2, \cdots)$ and the corresponding eigenvalues by λ_r; we shall omit an additional index p indicating the order of the density operator. The density matrix then has an eigenfunction expansion corresponding to the spectral resolution of Γ_p:

$$\Gamma_p(x,x')=\sum_r\lambda_r g_r(x)g_r^*(x'). \quad (3)$$

Because of the completeness of the g's, the wave function of the system can also be expanded in the form

$$\psi(x,y)=\binom{N}{p}^{-\frac{1}{2}}\sum_r g_r(x)h_r(y); \quad (4)$$

to each g_r we have thus associated a function h_r of $N-p$ variables defined by

$$h_r(y)=\binom{N}{p}^{\frac{1}{2}}\int dx\,g_r^*(x)\psi(x,y). \quad (5)$$

We shall now show that the different functions h_r are orthogonal:

$$(h_r,h_s)=\binom{N}{p}\int dy\int dx'\,g_r(x')\psi^*(x',y)$$

$$\times\int dx\,g_s^*(x)\psi(x,y)$$

$$=\int\int dxdx'\,g_s^*(x)\Gamma_p(x,x')g_r(x')$$

$$=\lambda_r\int dx\,g_s^*(x)g_r(x)$$

$$=\lambda_r\delta_{rs}. \quad (6)$$

---

[1] P. O. Löwdin, Phys. Rev. **97**, 1474 (1955).
[2] R. McWeeny, Revs. Modern Phys. **32**, 335 (1960).
[3] J. von Neumann, *Mathematical Foundations of Quantum Mechanics* (Princeton University Press, Princeton, New Jersey, 1955), pp. 188–191.

This result implies also that $h_r(y)$ vanishes identically for $\lambda_r=0$; only those g's that correspond to positive eigenvalues of Γ_p appear in the expansion (4) of the wave function. The h's that do not vanish are conveniently replaced by normalized functions

$$G_r(y)=\lambda_r^{-\frac{1}{2}}h_r(y) \quad (\lambda_r>0). \tag{7}$$

The expression (4) for the wave function now becomes

$$\psi(x,y)=\binom{N}{p}^{-\frac{1}{2}}\sum_r \lambda_r^{\frac{1}{2}}g_r(x)G_r(y). \tag{4a}$$

Because the g's are orthonormal, the density matrix of order $N-p$ can be written as

$$\Gamma_{N-p}(y,y')=\binom{N}{p}\int dx\,\psi(x,y)\psi^*(x,y')$$

$$=\sum_r \lambda_r G_r(y)G_r^*(y'). \tag{8}$$

This equation exhibits the spectral resolution of Γ_{N-p}: the G's are eigenfunctions of Γ_{N-p} and its spectrum of nonzero eigenvalues is identical with that of Γ_p.

In the preceding proof we have never had to ask how often zero occurs as an eigenvalue of either density operator. However, the answer is important in the discussion of two further questions: whether there is a unitary equivalence between the two density operators, as suggested by the equality of their positive eigenvalues; and, if there is, whether it can be proved by a method of polar decomposition. In both instances we try to define a unitary mapping of $\mathfrak{H}_{N-p}$ on $\mathfrak{H}_p$ by establishing a one-to-one correspondence in which each eigenfunction G_r of Γ_{N-p} corresponds to an eigenfunction g_r of Γ_p having the same eigenvalue. This procedure appears to be straightforward provided that only a finite number of positive eigenvalues occur. If there are an infinite number of positive eigenvalues—and examples can easily be constructed in which this is the case—there seems to be no guarantee that one can establish a one-to-one correspondence between the two subsets of eigenfunctions belonging to the eigenvalue zero. There need be no relation between their cardinal numbers, so far as we have been able to discover; it may even happen that an infinite number of G's and no g's at all belong to the eigenvalue zero. We shall now investigate further the special case of a finite number of positive eigenvalues, with the understanding that the results are not generally valid.

We assume that λ_r is positive for $r=1, 2, \cdots, m$ and zero for $r>m$. The functions $G_1, G_2, \cdots, G_m$ defined by Eqs. (5) and (7) are then the only eigenfunctions of Γ_{N-p} with positive eigenvalues (aside from their linear combinations in case of degeneracy). However, Γ_{N-p} has a complete orthonormal set of eigenfunctions in $\mathfrak{H}_{N-p}$, and those with zero eigenvalue may be selected in any order and denoted by $G_{m+1}, G_{m+2}, \cdots$. The

correspondence[4]

$$G_r \rightleftarrows g_r=SG_r \quad (r=1, 2, \cdots)$$

then defines a unitary mapping S of $\mathfrak{H}_{N-p}$ on $\mathfrak{H}_p$. The mapping and its inverse may be represented by integral operators with the kernels

$$S(x,y)=\sum_r g_r(x)G_r^*(y),$$
$$S^{-1}(y,x)=\sum_r G_r(y)g_r^*(x). \tag{9}$$

From Eqs. (3) and (8) we then obtain

$$\Gamma_{N-p}=S^{-1}\Gamma_p S. \tag{10}$$

Alternatively one may regard the wave function $\psi(x,y)$ as the kernel of an integral operator Ψ_p that maps $\mathfrak{H}_{N-p}$ on $\mathfrak{H}_p$. It is convenient first to define a unitary operator T by

$$g_r=TG_r^*, \quad (r=1, 2, \cdots)$$

$$g_r(x)=\int T(x,y)G_r^*(y)dy, \tag{11}$$

$$T(x,y)=\sum_r g_r(x)G_r(y).$$

We shall need also the transposed density operator $\tilde{\Gamma}_{N-p}$, defined by

$$\tilde{\Gamma}_{N-p}F(y)=\int \Gamma_{N-p}(y',y)F(y')dy'. \tag{12}$$

By use of Eqs. (3), (4a), and (8), we then obtain the (nonunique) polar decompositions

$$\Psi_p=\binom{N}{p}^{-\frac{1}{2}}\Gamma_p^{\frac{1}{2}}T=\binom{N}{p}^{-\frac{1}{2}}T\tilde{\Gamma}_{N-p}^{\frac{1}{2}}, \tag{13}$$

from which it follows that

$$\Gamma_p=\binom{N}{p}\Psi_p\Psi_p^{\dagger},$$

$$\tilde{\Gamma}_{N-p}=\binom{N}{p}\Psi_p^{\dagger}\Psi_p=T^{-1}\Gamma_p T. \tag{14}$$

Since Γ_{N-p} is Hermitian, it is unitarily equivalent to its transpose and thus, once again, to Γ_p.[5]

One might hope to relate the eigenvalues of density matrices of different orders by a quite different method, using the formalism of annihilation and creation oper-

[4] The g's (and likewise the G's) are countable because they form an orthonormal set in a Hilbert space of square-integrable functions of the particle coordinates. Such a space is separable and has a dimensionality that is denumerably infinite.

[5] We are indebted to Professor Klaus Ruedenberg for suggesting the polar decomposition as an alternative way of establishing the unitary equivalence. We have not been able to prove the existence of a polar decomposition of Ψ_p without essentially reproducing the steps that were used above to arrive at Eq. (8). It should be noted in this connection that Γ_p does not have an inverse.

ators. If a_1, a_2, $\cdots$ are the annihilation operators corresponding to a complete orthonormal set of one-particle states, density operators of successively lower orders can be obtained from

$$\Gamma_p = (N-p)^{-1} \sum_i a_i \Gamma_{p+1} a_i^\dagger. \qquad (15)$$

It is easy to verify that this relation is independent of the choice of basis, but not so easy to obtain useful information from it.

As one consequence of the theorem proved earlier in this paper, suppose one has a given function $K(x_1,x_2,x_1',x_2')$. A necessary condition for K to be a second-order density matrix for a 3-particle system is that the first-order density matrix obtained from K have the same positive eigenvalues as K itself. From the eigenfunctions, possible wave functions for the system could be constructed according to Eq. (4a). Likewise, knowledge of the eigenvalues of the second-

order density matrix of a 4-particle system gives extensive information about the wave function. In the latter case, for example, if the positive eigenvalues were nondegenerate, the wave function would necessarily be of the form

$$\psi = 6^{-\frac{1}{2}} \sum_r \lambda_r^{\frac{1}{2}} c_r g_r(1,2) g_r(3,4),$$

where the coefficients c_r have modulus unity. In the other extreme, where the density operator has six eigenfunctions with eigenvalue 1 and all other eigenvalues are zero, the wave function would be

$$\psi = 6^{-\frac{1}{2}} \sum_{r,s} c_{rs} g_r(1,2) g_s(3,4),$$

where the c's form a unitary matrix. The extra coefficients c appear in these last expressions because, without knowledge of the wave function, the functions G_r are indeterminate by a phase factor and, in the case of degenerate eigenvalues, by a unitary transformation.

Nonlinear Interaction of an Electromagnetic Wave with a Plasma Layer in the Presence of a Static Magnetic Field. I. Theory of Harmonic Generation*

R. F. Whitmer and E. B. Barrett
Palo Alto Laboratories, General Telephone and Electronics Laboratories, Palo Alto, California
(Received September 16, 1960)

The theory of electromagnetic wave propagation through an anisotropic ionized layer, including the effects of the nonlinear terms in the Boltzmann transport equation, is presented. The method of solution of the nonlinear equations involves an expansion of all of the dependent variables in a Fourier series in time. The differential equations describing wave propagation are then solved, for each frequency in the series, for plane wave propagation, including all of the reflections within the plasma layer. A solution in closed form has been obtained, under small signal conditions, for the field at the hth harmonic in the Fourier series. A discussion of the properties of the wave at the second harmonic frequency as a function of the dc magnetic field strength, the electron density, the electron-neutral particle collision frequency, the field strength of the incident wave, and the thickness of the plasma layer is given.

1. INTRODUCTION

THE propagation characteristics of an electromagnetic wave in the presence of an ionized medium have been discussed by Schlüter,[1,2] Bailey,[3-5] Spitzer,[6] Brown,[7] and many others.[8] These discussions are based upon a set of equations which includes Maxwell's equations and the dynamical equations for an ionized gas.

The dynamical equations are obtained, at least implicitly, from the Boltzmann equation, and they are inherently nonlinear equations. However, the usual procedure is to linearize these equations since a general method for obtaining solutions to the nonlinear equations is not available. It is the purpose of this paper to discuss the effects of the nonlinear terms in the equations on electromagnetic wave propagation phenomena.

Relatively little has been reported on solutions to these equations when the nonlinear terms are included. Ginsburg[9] has discussed the mixing of two electromagnetic waves when one of the waves, at frequency ω_1, causes an electron density gradient which varies at the ω_1 rate. The interaction of this electron density variation with a second electromagnetic wave, at frequency ω_2, is

---

[1] A. Schlüter, Z. Naturforsch. 5A, 72 (1950).
[2] A. Schlüter, Z. Naturforsch. 6A, 73 (1951).
[3] V. A. Bailey, J. Roy. Soc. N. S. W. 82, 107 (1948).
[4] V. A. Bailey, Australian J. Sci. Research A1, 351 (1948).
[5] V. A. Bailey, Phys. Rev. 78, 428 (1950).
[6] L. Spitzer, *Physics of Fully Ionized Gases* (Interscience Publishers, Inc., New York, 1956), Interscience Tracts on Physics and Astronomy, No. 3.
[7] S. C. Brown, *Handbuch der Physik*, edited by S. Flügge (Springer-Verlag, Berlin, 1956), Vol. XXII, p. 531.
[8] For an exhaustive list see "Bibliography on Plasma Physics and Magnetohydrodynamics," Engineering and Physical Sciences Library, University of Maryland, College Park, Maryland, 1959.

[9] V. L. Ginzburg, J. Exptl. Theoret. Phys. U.S.S.R. 35, 1573 (1958) [translation: Soviet Phys.—JETP 35(8), 1100 (1959)].