Slater Determinants and Quasiparticle Vacuum States Constructed from a Finite Number of Fermion States†*

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A theoretical study of single-particle transformations, quasiparticle transformations, Slater determinants, and quasiparticle vacuum states is made for a given finite number of single-fermion states. The usual unitary single-particle or quasiparticle transformations are generalized. The new transformations are the most general transformations which transform Slater determinants into Slater determinants or quasiparticle vacuum states into quasiparticle vacuum states, and they contain as particular cases Thouless's nonunitary transformation. It is shown that several Brillouin theorems used in Hartree-Fock and Hartree-Bogolubov variation theories follow from the form of the continuous variations which can be performed in the space of Slater determinants and in the space of quasiparticle vacuum states.

I. INTRODUCTION

SLATER determinants (SD) and quasiparticle vacuum states (QPVS) constructed from a finite number of fermion states are used in the Hartree-Fock and the Hartree-Bogoliubov variational methods applied to nuclear calculations.[1,2] The stability of the variational SD or QPVS solutions has been investigated in the literature with the aid of single-particle or quasiparticle unitary transformations,[2,3] and with the aid of nonunitary Thouless transformations.[2,4] The Thouless transformations proved advantageous because they do not contain redundant parameters.[2,4] However, the possibility of using both unitary and nonunitary Thouless transformations to study stability conditions, as well as the connection between these two kinds of transformations, has not been completely clarified hitherto.

In the present paper we introduce the most general single-particle and quasiparticle transformations, transforming a SD into a SD and a QPVS into a QPVS. We consider the Lie groups and the Lie algebras associated with these transformations in order to obtain the decomposition of a general transformation into a product containing a unitary transformation and a nonunitary Thouless-type transformation. It is shown, for instance, that the most general quasiparticle transformation, which conserves the anticommutation relations but not the relations of adjointness between fermion creation and annihilation operators, decomposes into a product of a generalized Bogoliubov (unitary) transformation, a diagonal, and a Thouless-type transformation.

We consider also the two spaces formed, respectively, by all the SD and by all the QPVS which can be constructed from the given single-fermion states. We determine the form of the continuous variations that can be performed in these two spaces. From the specific form of the variations and from the variational principles themselves, a number of theorems known as Brillouin theorems[2,5,6] and some criteria for choosing the "best" quasiparticle[6–8] can then easily be deduced. The usual derivations of these theorems, which make use of single-particle or quasiparticle transformations, are, in general, less direct and more involved.

II. SINGLE-PARTICLE TRANSFORMATIONS

Let us consider the $2n$ creation and annihilation operators

$$a_1^\dagger, \cdots, a_n^\dagger, \qquad a_1, \cdots, a_n, \tag{1}$$

corresponding to the given single-fermion states $a_1^\dagger|0\rangle$, $\cdots$, $a_n^\dagger|0\rangle$, and obeying the fermion anticommutation relations

$$[a_i^\dagger, a_j^\dagger]_+ = [a_i, a_j]_+ = 0, \tag{2}$$
$$[a_i^\dagger, a_j]_+ = \delta_{ij}.$$

It will be convenient to introduce the n-dimensional vector space V formed by the complex linear combination of the creation operators $a_i^\dagger$. A new basis of single-particle operators $b_i^\dagger$ of V may be obtained from the basis $a_i^\dagger$ by a unitary transformation. The $2n$ operators $b_i^\dagger$, b_i will then satisfy the fermion anticommutation relations (2).

A more general basis $b_i^\dagger$ of V may be obtained from the basis $a_i^\dagger$ by an invertible transformation T which

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is not necessarily unitary; i.e.,

$$b_i^\dagger = T a_i^\dagger T^{-1} = \sum_{j=1}^{n} T_{ij} a_j^\dagger . \qquad (3)$$

If T is not unitary, one has $[b_i^\dagger, b_j]_+ \neq \delta_{ij}$, but the creation operators $b_i^\dagger$ still anticommute among themselves:

$$b_i^\dagger b_j^\dagger = -b_j^\dagger b_i^\dagger . \qquad (4)$$

Relations (4) show that unnormalized Slater determinants

$$\prod_{i=1}^{N} b_i^\dagger \,|\, 0\rangle$$

can be constructed from the generalized operators (3) of V. In the following we shall mean by a SD a SD which is not necessarily normalized.

The invertible transformations T form a group G which is represented with respect to the basis $a_i^\dagger$ of V by the general complex matrix group $GL(n, C)$. Notice that a transformation T acts in two spaces: (i) in the operator space V following the rule $a_i^\dagger \rightarrow T a_i^\dagger T^{-1}$, and (ii) in the space of wave functions following the rule $|\Phi\rangle \rightarrow T|\Phi\rangle$. Since T is the most general transformation transforming creation operators into creation operators, it is also the most general transformation transforming SD's into SD's.

Let us consider now the three subgroups U, D, and N of G, which are isomorphic, respectively, to the unitary matrix group $U(n)$, the group of diagonal real matrices, and the group formed by the complex upper triangular matrices with ones on the main diagonal. It was shown[9] that a transformation belonging to a connected group can be written as a product of terms of the form e^t, where t is a Lie-algebra element. Since the groups G, U, D, and N are connected, it will be sufficient to determine their Lie algebras L_g, L_u, L_d, and L_n.

The Lie algebra of $GL(n, C)$ consists of all $n \times n$ complex matrices, and a basis is formed by the matrices E_{jk} with 1 at the intersection of the j row and k column and 0 everywhere else. With respect to the basis $a_i^\dagger$ of V, the n^2 operators $a_j^\dagger a_k$ are represented by the matrices E_{jk}. Hence, an arbitrary element of the Lie algebra L_g may be written

$$t_g = \sum_{j,k} c_{jk} a_j^\dagger a_k, \qquad (5)$$

where c_{jk} are complex coefficients. Since the Lie algebra L_u contains only anti-Hermitian operators, an arbitrary element of L_u has the form

$$t_u = i \sum_{j>k} (m_{jk} a_j^\dagger a_k + m_{jk}^* a_k^\dagger a_j) + i \sum_j m_j a_j^\dagger a_j, \qquad (6)$$

where the m_{jk} are complex and the m_j are real. It can be verified also that an arbitrary element of L_d is given by

$$t_d = \sum_j s_j a_j^\dagger a_j, \qquad (7)$$

where the s_j are real, and that an arbitrary element of L_n has the form

$$t_n = \sum_{j>k} p_{jk} a_j^\dagger a_k, \qquad (8)$$

where the p_{jk} are complex.

The decomposition

$$t_g = t_u + t_d + t_n \qquad (9)$$

is now readily obtained by comparing the scalar coefficients on both sides of Eq. (9). The corresponding decomposition for transformations T of the group G is written

$$T = T_u T_d T_n, \qquad (10)$$

where $T_u = e^{t_u}$, $T_d = e^{t_d}$, and $T_n = e^{t_n}$, and is a particular case of the general Iwasawa decomposition.[9]

A Thouless transformation is given by[4]

$$T_{\mathrm{Th}} = \exp\Big(\sum_{j>N} \sum_{k\leq N} p_{jk} a_j^\dagger a_k\Big) = \prod_{j>N, k\leq N} (1 + p_{jk} a_j^\dagger a_k), \qquad (11)$$

where the indices $k = 1, \cdots, N$, and $j = N+1, \cdots, n$, stand, respectively, for the occupied and the unoccupied states in the trial SD. It is clear that T_{Th} is a particular case of the transformation T_n, which has the form

$$T_n = \exp\Big(\sum_{j>k} p_{jk} a_j^\dagger a_k\Big). \qquad (12)$$

The connection between unitary and Thouless transformations is thus established: Both kinds of transformations are components in the standard decomposition (10) of the general transformations T.

III. SLATER DETERMINANTS

Following our convention of Sec. II, it can now be said that N generalized creation operators $b_1^\dagger, \cdots, b_N^\dagger$, define up to a scalar factor a SD

$$\prod_{i=1}^{N} b_i^\dagger \,|\, 0\rangle.$$

However, the SD

$$\prod_{i=1}^{N} b_i^\dagger \,|\, 0\rangle$$

does not specify uniquely the set of operators $b_1^\dagger, \cdots, b_N^\dagger$, because new creation operators

$$d_i^\dagger = \sum_{j=1}^{N} S_{ij} b_j^\dagger, \qquad i = 1, \cdots, N \qquad (13)$$

define the same SD up to the scalar factor $\det|S_{ij}|$. The correct statement is, in this case, that a SD specifies uniquely an N-dimensional subspace V_N of the space V spanned by $b_1^\dagger, \cdots, b_N^\dagger$. This establishes a one-to-one correspondence between SD's defined up to a scalar factor and N-dimensional subspaces V_N of V.

[9] R. Hermann, *Lie Groups for Physicists* (W. A. Benjamin, Inc., New York, 1966).

The above correspondence may be used to determine the number of essential parameters necessary to specify a SD with respect to the given basis $a_i^\dagger$ of V. An N-dimensional subspace V_N of V is completely determined by giving a system of $n-N$ homogeneous linear equations with n unknowns

$$\sum_{j=1}^{n} A_{ij}x_j=0, \qquad i=1, \cdots, n-N. \tag{14}$$

This system may be solved for the first $n-N$ unknowns

$$x_i=\sum_{j>n-N} B_{ij}x_j, \qquad i=1, \cdots, n-N; \tag{15}$$

hence it involves only $N(n-N)$ complex parameters B_{ij}. A SD is therefore specified up to a scalar factor by $N(n-N)$ essential complex parameters. This is exactly the number of parameters involved in a Thouless transformation [cf. Eq. (11)].

We denote now by K_N the space formed by all the Slater determinants of order N which can be constructed from the creation operators of the space V. It is clear that K_N is not a vector space, because a linear combination $\alpha\,|\,\Phi\rangle+\beta\,|\,\Phi'\rangle$ of two SD's is not, in general, a SD. It can be verified without difficulty that such a linear combination is a SD if and only if the two SD's differ by at most one excitation; i.e., a basis $b_i^\dagger$ of V can be found such that

$$|\,\Phi\rangle=b_1^\dagger b_2^\dagger\cdots b_N^\dagger\,|\,0\rangle, \qquad |\,\Phi'\rangle=b_m^\dagger b_2^\dagger\cdots b_N^\dagger\,|\,0\rangle. \tag{16}$$

It follows that an elementary continuous variation in the space K_N has the form

$$\delta\,|\,\Phi\rangle=\epsilon_1\,|\,\Phi\rangle+\epsilon_2 b_m^\dagger b_i\,|\,\Phi\rangle, \qquad m>N,\ i\leq N, \tag{17}$$

where the scalars ϵ_1 and ϵ_2 take care, respectively, of the variations of the SD $|\,\Phi\rangle$ and of its once-excited component $b_m^\dagger b_i\,|\,\Phi\rangle$.

The Hartree-Fock theory is based on the variational principle

$$\delta\langle H\rangle=0, \tag{18}$$

where $\langle H\rangle=\langle\Phi\,|\,H\,|\,\Phi\rangle/\langle\Phi\,|\,\Phi\rangle$, and the variation of $|\,\Phi\rangle$ has to be performed continuously in the space K_N. The variational principle is not sensitive to the first kind of continuous variation, $\delta_1\,|\,\Phi\rangle=\epsilon_1\,|\,\Phi\rangle$, because of the identity

$$\delta_1\langle H\rangle=\frac{\langle\delta_1\Phi\,|\,H\,|\,\Phi\rangle}{\langle\Phi\,|\,\Phi\rangle}-\frac{\langle\Phi\,|\,H\,|\,\Phi\rangle\langle\delta_1\Phi\,|\,\Phi\rangle}{\langle\Phi\,|\,\Phi\rangle^2} =0. \tag{19}$$

The stationarity of $\langle H\rangle$ with respect to all the possible continuous variations of the second kind $\delta_2\,|\,\Phi\rangle=\epsilon_2 b_m^\dagger b_i\,|\,\Phi\rangle$ leads to the equations

$$\langle\Phi\,|\,b_i^\dagger b_m H\,|\,\Phi\rangle=\langle\Phi\,|\,Hb_m^\dagger b_i\,|\,\Phi\rangle=0, \tag{20}$$

which state the well-known Brillouin theorem.[5] The Brillouin theorem may thus be seen as a consequence of the topological structure of the space K_N.

The Thouless transformations (11) perform only continuous variations of the second kind on the SD

$$\prod_{i=1}^{N} a_i^\dagger\,|\,0\rangle.$$

Thus, they do not involve redundant parameters and are more adequate for the study of the stability conditions.

IV. QUASIPARTICLE TRANSFORMATIONS

In this section, we introduce quasiparticle transformations more general than the usual generalized Bogoliubov transformations,[1] and we show that the new transformations contain as a particular case the generalized Thouless transformations.[4]

Let us consider the complex vector space W spanned by the $2n$ fermion operators $a_1^\dagger, \cdots, a_n^\dagger$, and $a_1, \cdots, a_n$. These operators obey the anticommutation relations (2) and satisfy the relations of adjointness, i.e., the $a_i^\dagger$ are Hermitian conjugates of the a_i, and

$$a_i=(a_i^\dagger)^\dagger. \tag{21}$$

The anticommutation relations (2) may be interpreted[10] as defining a bilinear symmetric form in the space W. The $2n$ operators

$$h_j=\tfrac{1}{2}\sqrt{2}(a_j^\dagger+a_j), \qquad h_{n+j}=\tfrac{1}{2}i\sqrt{2}(a_j^\dagger-a_j), \qquad j=1, \cdots, n, \tag{22}$$

whose anticommutation relations read

$$[h_j, h_k]_+=\delta_{jk}, \tag{23}$$

form an orthonormal basis of W with respect to the bilinear form. The relations (21) become in this basis

$$h_j^\dagger=h_j. \tag{24}$$

We are now interested in finding the explicit form of transformations S, which conserve only fermion anticommutation relations, and, also, of generalized Bogoliubov transformations S_{B}, which conserve both relations (2) and (20).

It has been shown[10,11] that the group O_{B} of Bogoliubov transformations S_{B} is isomorphic to the group $O(2n, R)$ of real orthogonal matrices. The group O formed by the transformations S is the most general group leaving invariant the bilinear symmetric form of the complex space W; it is therefore isomorphic to the complex orthogonal matrix group $O(2n, C)$.

We shall determine first the form of the transformations S' and S_{B}' belonging to the subgroups O' and O_{B}' of O and O_{B}, which are isomorphic to $SO(2n, C)$ and $SO(2n, R)$. Since they belong to connected groups, the transformations O' and O_{B}' may be written as one

[10] A. K. Bose and A. Navon, Phys. Letters **17**, 95 (1965).
[11] C. Bloch and A. Messiah, Nucl. Phys. **39**, 95 (1962).

term, or as a product of terms of the form e^s, where s is a Lie-algebra element.[9] A Lie-algebra element s acts in the space W, following the rule

$$a_j \to [s, a_j]_- . \quad (25)$$

Let us consider now the $n(2n-1)$ elements of the form $h_j h_k$ ($j<k=1, \cdots, 2n$). These elements are linearly independent, generate by commutation a closed space, and map any element of W, according to the rule (24), into another element of W. An element s of the Lie algebra L of O' must be antisymmetric with respect to transposition, while an element s_B of the Lie algebra L_B of O_B' must be both antisymmetric and real. For operators expressed in second quantization notation, the operation of transposition has to be defined, with respect to the bilinear form represented in W by the anticommutator. One obtains from this definition that the transpose of a product of operators h_j, or $a_j^\dagger$, a_j, is the product of the same operators written in reversed order. Hence,

$$(h_j h_k)^t = h_k h_j = -h_j h_k, \quad (26)$$

and the operators $h_j h_k$ thus form a basis for the Lie algebras L and L_B. Arbitrary elements s and s_B may now be written in the form

$$\sum_{j<k} m_{jk} h_j h_k,$$

where the coefficients m_{jk} are complex for s and real for s_B. In terms of the operators $a_j^\dagger$, a_j, the elements s and s_B may be expressed as follows:

$$s = \sum_{j<k} (m_{jk} a_j^\dagger a_k^\dagger + n_{jk} a_j a_k) + \sum_{j\neq k} p_{jk} a_j^\dagger a_k + \sum_j r_j (2a_j^\dagger a_j - 1), \quad (27)$$

$$s_B = \sum_{j<k} [m_{jk}'(a_j^\dagger a_k^\dagger - a_k a_j) + i n_{jk}'(a_j^\dagger a_k^\dagger + a_k a_j) + p_{jk}'(a_j^\dagger a_k - a_k^\dagger a_j) + i q_{jk}'(a_j^\dagger a_k + a_k^\dagger a_j)] + \sum_j i r_j'(2a_j^\dagger a_j - 1), \quad (28)$$

where the primed coefficients are restricted to be real.

From the isomorphism between the groups O, O_B and the groups $O(2n, C)$, $O(2n, R)$, we can assert now that a transformation S or S_B is either proper, or can be written as a product of a chosen reflection and a proper transformation. In order to know the general expression of a transformation S or S_B, it will be sufficient to determine the form of some reflection. If we put

$$R = \sqrt{2} h_i = a_i^\dagger + a_i, \quad (29)$$

and notice that

$$R^{-1} = R, \quad (30)$$

it follows that the basis vectors h_j of W transform like

$$h_i \to R h_i R^{-1} = h_i, \qquad h_j \to R h_j R^{-1} = -h_j \qquad (j \neq i), \quad (31)$$

and R is thus clearly a reflection.

We show now that a transformation S can be decomposed in a unique way into a product containing a Bogoliubov and a Thouless-type transformation. We remark first that the arbitrary elements s and s_B of the Lie algebras L and L_B may also be expressed by replacing in Eqs. (27) and (28), the particle operators $a_i^\dagger$, a_i, by quasiparticle operators $c_i^\dagger$, c_i. Let us introduce at this point the following Lie algebras: (i) the commutative Lie algebra H_d spanned by the diagonal elements

$$s_d = \sum_{i=1}^{n} s_i (2c_i^\dagger c_i - 1), \quad (32)$$

where s_i are real parameters; and, (ii) the nilpotent Lie algebra H_n spanned by the elements

$$s_n = \sum_{j>k} (p_{jk} c_j^\dagger c_k^\dagger + r_{jk} c_j^\dagger c_k), \quad (33)$$

where p_{jk}, r_{jk} are complex parameters.

It can be verified without difficulty that an element s expressed in terms of $c_i^\dagger$, c_i can be decomposed in a unique way as

$$s = s_B + s_d + s_n. \quad (34)$$

It follows that a group transformation can be expressed in the form

$$S = S_B S_d S_n, \quad (35)$$

where $S_d = e^{s_d}$ and $S_n = e^{s_n}$. A generalized Thouless transformation is given by[4]

$$S_{Th} = \exp(\sum_{j>k} p_{jk} c_j^\dagger c_k^\dagger). \quad (36)$$

It is clear that S_{Th} is a particular case of S_n. Thus, the quasiparticle transformations S we have introduced contain as components generalized Bogoliubov and generalized Thouless transformations.

V. QUASIPARTICLE VACUUM STATES

A quasiparticle vacuum state $|\Phi\rangle$ is usually defined in one of two ways:

(i) There exist n annihilation quasiparticle operators $c_i = S_B a_i S_B^{-1}$, which satisfy the relations

$$c_i |\Phi\rangle = 0; \quad (37)$$

(ii) $|\Phi\rangle$ may be expressed in the form

$$|\Phi\rangle = S_B |0\rangle. \quad (38)$$

These definitions can be generalized by replacing the Bogoliubov transformations S_B by the more general transformations S introduced in the previous section. This is possible because the set of quasiparticle operators c_i defining $|\Phi\rangle$ in (i) is characterized only by the anticommutation relations

$$[c_i, c_j]_+ = 0, \quad (39)$$

and does not imply relations of adjointness. Thus, any

QPVS may be written in the form

$$|\Phi\rangle = S|0\rangle. \quad (40)$$

From the definition of a QPVS it follows that n anticommuting quasiparticle operators $c_1, \cdots, c_n$ define a QPVS $|\Phi\rangle$ up to a multiplicative constant. However, the QPVS $|\Phi\rangle$ defines uniquely only the n-dimensional complex space W_n spanned by the operators $c_1, \cdots, c_n$. W_n is a subspace of W such that any of its elements x satisfies the relation

$$[x, x]_+ = 0. \quad (41)$$

Such a subspace is called isotropic. The correspondence between the QPVS's and the isotropic subspaces of W was studied in the frame of the algebraic theory of spinors.[12]

We shall denote by K the space formed by all the QPVS's. It was seen in Sec. IV that a transformation S is either proper, or can be written as a product of a reflection and a proper transformation. Proper transformations applied on the particle vacuum $|0\rangle$ generate QPVS's with an even parity of the particle number, while improper transformations generate QPVS's which have an odd parity of the particle number. Hence, the space K is the direct sum

$$K = K_e \dot{+} K_0 \quad (42)$$

of two connected spaces K_e and K_0, containing, respectively, the even and the odd QPVS's. One cannot pass from K_e to K_0 by a continuous variation, but only by a reflection.

It was proved in Ref. 10 that a linear combination $\alpha|\Phi\rangle + \beta|\Phi'\rangle$ of two QPVS $|\Phi\rangle$ and $|\Phi'\rangle$ is a QPVS only if the isotropic subspaces W_n and W_n' defining $|\Phi\rangle$ and $|\Phi'\rangle$ have an intersection of dimension n or $(n-2)$. This implies, in second-quantization language, that $|\Phi\rangle$ and $|\Phi'\rangle$ must be proportional, or must differ by two quasiparticle excitations. It follows that an elementary continuous variation of a QPVS $|\Phi\rangle$ defined by the annihilation quasiparticle operators c_i has the form

$$\delta|\Phi\rangle = \epsilon_1|\Phi\rangle + \epsilon_2 c_m^\dagger c_n^\dagger |\Phi\rangle, \quad (43)$$

where ϵ_1, ϵ_2 are coefficients corresponding to two kinds of variation.

Hartree-Bogoliubov theory is based on the variational principle (18), where $\langle H\rangle$ is now varied with respect to wave functions $|\Phi\rangle$ in K. As in the Hartree-Fock theory, the variational principle is not sensitive to variations $\delta_1|\Phi\rangle = \epsilon_1|\Phi\rangle$ of the first kind. The stationarity of $\langle H\rangle$ with respect to variations $\delta_2|\Phi\rangle = \epsilon_2 c_m^\dagger c_n^\dagger|\Phi\rangle$ of the second kind yields the Brillouin-Bogoliubov (BB) equations[6]

$$\langle\Phi|c_n c_m H|\Phi\rangle = \langle\Phi|H c_m^\dagger c_n^\dagger|\Phi\rangle = 0. \quad (44)$$

These equations are thus a consequence of the topological structure of the space K.

The generalized Thouless transformations (36) can also be written

$$S_{\mathrm{Th}} = \prod_{j>k} (1 + p_{jk} c_j^\dagger c_k^\dagger). \quad (45)$$

It is seen that, in this form, these transformations perform exclusively variations of the second kind on the QPVS $|\Phi\rangle$, and therefore do not contain redundant parameters.

The structure of the continuous variations in the space K is also responsible for the equivalence of criteria for choosing the best quasiparticle.[7] Thus, it was proved[6–8] that the criterion of maximum overlap

$$\delta(\mathrm{Re}\langle\Psi|\Phi\rangle) = 0, \quad (46)$$

where $|\Psi\rangle$ is the true ground state and $|\Phi\rangle$ is the trial QPVS, is equivalent to the principle of compensation of dangerous diagrams of Bogoliubov:

$$\delta(\mathrm{Re}\langle\Psi|c_i^\dagger c_j^\dagger|\Phi\rangle) = \delta(\mathrm{Re}\langle\Psi|c_i c_j|\Phi\rangle) = 0. \quad (47)$$

The proof of this equivalence was quite involved, while here it appears simply as a consequence of the topological structure of the space K.

VI. CONCLUSIONS

The main result obtained in this work is the introduction, in Secs. II and IV, of single-particle and quasiparticle nonunitary transformations. The decomposition of these transformations in terms of unitary and Thouless transformations illustrates the connection, hitherto unknown, between these last two kinds of transformation.

In Secs. III and V the spaces of Slater determinants and of quasiparticle vacuum states are studied as entities, rather than through the intermediary of single-particle or quasiparticle transformations. It is seen thus, that the topological structure of these spaces is directly responsible for several properties of the variational Hartree-Fock and Hartree-Bogoliubov methods.

This work can be seen as a generalization of the usual single-particle and quasiparticle methods. Several particular results may also be applied to specific problems, such as the study of stability conditions and the treatment of neutron-proton correlations with the aid of quasiparticle transformations.

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[12] C. Chevalley, *The Algebraic Theory of Spinors* (Columbia University Press, New York, 1954).