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Diagonalisation of the quadratic fermion Hamiltonian with a linear part

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Abstract. It is well known that the spectrum of a *homogeneous* quadratic Hamiltonian in m fermion construction-operator pairs is characterised by m mode energies. In this paper it is proved that the spectrum of a quadratic Hamiltonian with a linear part presents the same feature. Simple methods are given for the calculation of the mode energies and of the ground-state energy of the Hamiltonian. It is shown that, in contrast to the boson case, the diagonalisation cannot be carried out by a *linear* transformation of the fermion construction operators. Application of such a transformation can only result in a diagonalisation after the introduction of a 'ghost' particle (fermion) and a corresponding pair of Hermitian-conjugate construction operators.

1. Introduction

In a previous paper (Colpa 1978), to which we shall refer as C, we discussed the diagonalisation of homogeneous quadratic expressions in a finite set of construction operators†. It was seen that for the solution of that (quasi-particle) problem it is quite possible to consider the boson and fermion cases as counterpart problems. The treatment of the properties of both types of construction operators with respect to their creation and destruction of *real* particles can also be kept strictly parallel (see for example de Boer 1965). Such a treatment, however, is certainly not possible for all problems. As an example we consider in this paper the diagonalisation of a Hamiltonian of the general form (m denotes an arbitrary positive integer):

$$\mathbf{H} \equiv \sum_{r',r=1}^{m} (\boldsymbol{\alpha}_{r'}^{\dagger} D_{1r'r} \boldsymbol{\alpha}_r + \boldsymbol{\alpha}_{r'}^{\dagger} D_{2r'r} \boldsymbol{\alpha}_r^{\dagger} + \boldsymbol{\alpha}_{r'} D_{3r'r} \boldsymbol{\alpha}_r + \boldsymbol{\alpha}_{r'} D_{4r'r} \boldsymbol{\alpha}_r^{\dagger}) + \sum_{r=1}^{m} (M_r \boldsymbol{\alpha}_r + M_r^* \boldsymbol{\alpha}_r^{\dagger}), \tag{1.1}$$

which is a quadratic expression with a linear part in a finite set of fermion construction operators $\boldsymbol{\alpha}_r$, $\boldsymbol{\alpha}_r^{\dagger}$; the coefficients $D_{ir'r}$ ($i = 1, 2, 3, 4$) and M_r can be complex numbers. Linear parts in fermion-operator Hamiltonians can occur quite well in physical theories, e.g. at a transition from observables to construction operators. For instance, one encounters linear (and higher odd-degree) terms in the frequently considered anisotropic XY-model (see e.g. Lieb *et al* 1961) after the application of a magnetic field parallel to the X- or Y-axis (or parallel to some other direction in the XY-plane).

† After de Boer (1965) we use the term 'construction operators' to denote boson and fermion creation and annihilation operators.

The counterpart problem, the diagonalisation of a Hamiltonian of the form (1.1) with all $\boldsymbol{\alpha}$ representing boson construction operators, has often been considered in the literature. In that case the diagonalisation is straightforward. In a first step applying § 4 of C, one carries out a homogeneous linear transformation which turns the set of boson construction operators $\boldsymbol{\alpha}$ into another such set of $\boldsymbol{\beta}$ and which diagonalises the homogeneous quadratic part according to:

$$\sum_{r',r=1}^{m} (\boldsymbol{\alpha}_{r'}^{\dagger} D_{1r'r} \boldsymbol{\alpha}_r + \boldsymbol{\alpha}_{r'}^{\dagger} D_{2r'r} \boldsymbol{\alpha}_r^{\dagger} + \boldsymbol{\alpha}_{r'} D_{3r'r} \boldsymbol{\alpha}_r + \boldsymbol{\alpha}_{r'} D_{4r'r} \boldsymbol{\alpha}_r^{\dagger}) = \sum_{r=1}^{m} 2\lambda_r \boldsymbol{\beta}_r^{\dagger} \boldsymbol{\beta}_r + \text{constant} \tag{1.2}$$

(we keep the coefficient 2 before λ_r in view of later developments in this paper). Since under such a transformation the linear part remains linear, the full Hamiltonian (1.1) can be expressed in terms of these new construction operators $\boldsymbol{\beta}_r$, $\boldsymbol{\beta}_r^{\dagger}$ as (note that $\mathbf{H}$ is a Hermitian operator):

$$\mathbf{H} = \sum_{r=1}^{m} \mathbf{H}_r + \text{constant}, \qquad \mathbf{H}_r \equiv 2\lambda_r \boldsymbol{\beta}_r^{\dagger} \boldsymbol{\beta}_r + \mu_r \boldsymbol{\beta}_r + \mu_r^* \boldsymbol{\beta}_r^{\dagger},$$

$$\lambda_r \text{ real}^{\dagger} \text{ numbers}, \ \mu_r \text{ complex numbers}. \tag{1.3}$$

Now a 'translation' transformation from the operators $\boldsymbol{\beta}$ to operators $\boldsymbol{\gamma}$ according to:

$$\boldsymbol{\beta}_r = \boldsymbol{\gamma}_r + t_r, \qquad \boldsymbol{\beta}_r^{\dagger} = \boldsymbol{\gamma}_r^{\dagger} + t_r^*, \qquad t_r \text{ complex numbers}, \quad r = 1, 2, \ldots, m, \tag{1.4}$$

does not affect the commutation relations for boson operators. By this transformation the terms $\mathbf{H}_r$ in equation (1.3) pass into:

$$\mathbf{H}_r = 2\lambda_r \boldsymbol{\gamma}_r^{\dagger} \boldsymbol{\gamma}_r + (2\lambda_r t_r^* + \mu_r) \boldsymbol{\gamma}_r + (2\lambda_r t_r + \mu_r^*) \boldsymbol{\gamma}_r^{\dagger} + (2\lambda_r |t_r|^2 + \mu_r t_r + \mu_r^* t_r^*), \tag{1.5}$$

and we see by inspection that (in case all $\lambda_r \neq 0$) the choice $t_r = -\mu_r^*/2\lambda_r$ transforms away the linear part of the $\mathbf{H}_r$. So we obtain:

$$\mathbf{H} = \sum_{r=1}^{m} (2\lambda_r \boldsymbol{\gamma}_r^{\dagger} \boldsymbol{\gamma}_r - |\mu_r|^2/2\lambda_r) \equiv \sum_{r=1}^{m} \hbar\omega_r \boldsymbol{\gamma}_r^{\dagger} \boldsymbol{\gamma}_r + \text{constant}. \tag{1.6}$$

As is well known the eigenvalues E of the Hamiltonian can be read immediately from the form of equation (1.6). The eigenvalues of $\mathbf{H}$ are given by:

$$E = \sum_{r=1}^{m} 2n_r \lambda_r + \text{constant} \equiv \sum_{r=1}^{m} n_r \hbar\omega_r + \text{constant}, \tag{1.7}$$

where each n_r can assume any non-negative integer. We express this situaton concisely by saying that the spectrum of a quadratic m-mode (i.e. m boson-operator pairs are involved) boson Hamiltonian with a linear part is characterised by the m mode energies $\hbar\omega_r \equiv 2\lambda_r$. Note that the values of the mode energies of a homogeneous quadratic boson Hamiltonian are not affected if one adds a linear part to that Hamiltonian.

In this paper we prove that also in case the $\boldsymbol{\alpha}$ in equation (1.1) are fermion operators, the spectrum of the Hamiltonian is characterised by m mode energies, i.e. the eivenvalues E of the Hamiltonian are again given by an equation of the form (1.7) where now the n_r can assume only the values 0 and 1. If one tries to prove this in a similar way as done above for the boson case, we immediately encounter the first

† Strictly speaking the considerations of C were more restricted than is suggested here: in the resulting diagonalised expression all λ_r were positive. In what follows we do not want this restriction on the λ_r and we consider equation (1.3) with arbitrary real λ_r.

difficulty that, even for $m = 1$, a transformation of the form (1.4) does not conserve the *anti*commutation relations for fermion operators. In § 4 it is shown that in general non-linear transformations are involved in the diagonalisations. For $m > 1$ we are faced with a second difficulty, in that by the validity of the anticommutation relations the terms $\mathbf{H}_r$ in equation (1.3) do not commute in general, whereas the terms $\hbar\omega_r\boldsymbol{\gamma}_r^\dagger\boldsymbol{\gamma}_r$ do in the final expression (1.6). In view of this we may expect that in the fermion case each particular mode energy is usually a function of all λ_r and μ_r.

At this stage it is evident that one cannot gain much advantage from the viewpoint that bosons and fermions constitute counterpart problems in mathematics. Of course one can use a brute-force method and diagonalise with the help of a computer the (Hermitian) 2^m-square matrix which represents the Hamiltonian $\mathbf{H}$. For $m = 3$ for example, if in the occupation-number representation the order of rows and columns is given by the order of the $2^3 = 8$ basis vectors:

$$|000\rangle, |100\rangle, |010\rangle, |110\rangle, |001\rangle, |101\rangle, |011\rangle, |111\rangle, \tag{1.8}$$

the Hamiltonian (1.3) is represented by (we omit the additive constant):

$$\mathbf{H} \equiv \mathbf{H}_1 + \mathbf{H}_2 + \mathbf{H}_3 \equiv$$

$$\begin{pmatrix}
0 & \mu_1 & \mu_2 & 0 & \mu_3 & 0 & 0 & 0 \\
\mu_1^* & 2\lambda_1 & 0 & -\mu_2 & 0 & -\mu_3 & 0 & 0 \\
\mu_2^* & 0 & 2\lambda_2 & \mu_1 & 0 & 0 & -\mu_3 & 0 \\
0 & -\mu_2^* & \mu_1^* & 2(\lambda_1+\lambda_2) & 0 & 0 & 0 & \mu_3 \\
\mu_3^* & 0 & 0 & 0 & 2\lambda_3 & \mu_1 & \mu_2 & 0 \\
0 & -\mu_3^* & 0 & 0 & \mu_1^* & 2(\lambda_1+\lambda_3) & 0 & -\mu_2 \\
0 & 0 & -\mu_3^* & 0 & \mu_2^* & 0 & 2(\lambda_2+\lambda_3) & \mu_1 \\
0 & 0 & 0 & \mu_3^* & 0 & -\mu_2^* & \mu_1^* & 2(\lambda_1+\lambda_2+\lambda_3)
\end{pmatrix} \tag{1.9}$$

It is seen that already for very small values of m one is confronted with rather large matrices; their construction has to be performed very carefully and, still worse, one does not recognise from them that the spectrum can be characterised by m mode energies. Since to our knowledge this characteristic of the spectrum of a fermion Hamiltonian of the form (1.1) has never been proved generally, for the time being we may even doubt that the spectrum possesses this property.

This paper is organised as follows. In § 2 we solve completely generally the problem of the diagonalisation of a fermion Hamiltonian of the form (1.1). By the introduction of a 'ghost' particle we are able to reduce the problem to the diagonalisation of a *homogeneous* quadratic fermion Hamiltonian, which can be solved by the standard method presented in Appendix A of this paper. Thus we show that the spectrum of equation (1.1) can indeed be characterised by m mode energies, and that one can find these energies by the unitary diagonalisation of an Hermitian matrix of order only $2(m+1)$; this order is to be compared with the order 2^m of matrices like (1.9). Also the ground-state energy will be calculated. Applying a procedure of Lieb *et al* (1961) we show in § 3 that, in case all coefficients in the Hamiltonian (1.1) are real, one can find the mode energies by the (orthogonal) diagonalisation of a symmetric real matrix of order m. In § 4 the direct relation is discussed between the original construction operators $\boldsymbol{\alpha}$ and new ones $\boldsymbol{\gamma}$, in terms of which the Hamiltonian (1.1) can be written in the form (1.6); it is made plausible that in general such a direct relation is too complicated to be of any

practical use. We summarise the results of this paper in § 5. In Appendix B a theorem is proved which is used in the Appendix A already mentioned, in Appendix C we discuss a detail occurring in our treatment.

2. Diagonalisation of the fermion Hamiltonian (1.1) by homogenisation. General method

In this section we shall first convert the fermion Hamiltonian (1.1) in such a way that it can be tackled by standard methods and thereafter we shall carry out the actual diagonalisation. According to Appendix A (equation (A.4)) we can assume without restricting the generality that the $2m$-square matrix

$$\mathscr{D} \equiv \begin{pmatrix} D_1 & D_2 \\ D_3 & D_4 \end{pmatrix} \equiv \begin{pmatrix} A & B \\ -B^* & -A^* \end{pmatrix} \tag{2.1}$$

has the form shown in equation (2.1) and is Hermitian. In accordance with Appendix A we call $\mathscr{D}$ the grand-dynamical matrix of the homogeneous quadratic part of equation (1.1). Assuming that the relevant Hilbert space $\mathscr{H}$ has the dimension 2^m (in the following treatment it is allowed that an arbitrary number of the m construction-operator pairs do not occur explicitly in the Hamiltonian (1.1) because of zero coefficients), we introduce a 2^{m+1}-dimensional Hilbert space $\tilde{\mathscr{H}}$ by the introduction of a 'ghost' particle. In addition to the m pairs† $\tilde{\boldsymbol{\alpha}}_r, \tilde{\boldsymbol{\alpha}}_r^\dagger$ $(r = 1, 2, \ldots, m)$ let an $(m+1)$-th fermion construction-operator pair $\tilde{\boldsymbol{\alpha}}_0, \tilde{\boldsymbol{\alpha}}_0^\dagger$ be defined in $\tilde{\mathscr{H}}$, which corresponds to the first occupation number occurring in the occupation-number representation of the basis kets $|n_0 n_1 n_2 \ldots n_m\rangle$ of $\tilde{\mathscr{H}}$ ($n_r = 0$ or 1; $r = 0, 1, 2, \ldots, m$). Now we homogenise the Hamiltonian (1.1), i.e. we define in the larger Hilbert space a *homogeneous* quadratic Hamiltonian $\tilde{\mathbf{H}}$ which is constructed from the Hamiltonian (1.1) by substituting *in the linear part*:

$$\boldsymbol{\alpha}_r \to \tilde{\boldsymbol{\alpha}}_0^\dagger \tilde{\boldsymbol{\alpha}}_r - \tilde{\boldsymbol{\alpha}}_0 \tilde{\boldsymbol{\alpha}}_r, \qquad \boldsymbol{\alpha}_r^\dagger \to \tilde{\boldsymbol{\alpha}}_r^\dagger \tilde{\boldsymbol{\alpha}}_0 - \tilde{\boldsymbol{\alpha}}_r^\dagger \tilde{\boldsymbol{\alpha}}_0^\dagger, \tag{2.2}$$

whereas *the quadratic part* is left unchanged apart from adding tildes to denote that the construction operators are now defined in $\tilde{\mathscr{H}}$. Thus we obtain:

$$\tilde{\mathbf{H}} = \sum_{r',r=1}^{m} \{\tilde{\boldsymbol{\alpha}}_{r'}^\dagger D_{1r'r} \tilde{\boldsymbol{\alpha}}_r + \tilde{\boldsymbol{\alpha}}_{r'}^\dagger D_{2r'r} \tilde{\boldsymbol{\alpha}}_r^\dagger + \tilde{\boldsymbol{\alpha}}_{r'} D_{3r'r} \tilde{\boldsymbol{\alpha}}_r + \tilde{\boldsymbol{\alpha}}_{r'} D_{4r'r} \tilde{\boldsymbol{\alpha}}_r^\dagger\}$$

$$+ \sum_{r=1}^{m} \{M_r (\tilde{\boldsymbol{\alpha}}_0^\dagger \tilde{\boldsymbol{\alpha}}_r - \tilde{\boldsymbol{\alpha}}_0 \tilde{\boldsymbol{\alpha}}_r) + M_r^* (\tilde{\boldsymbol{\alpha}}_r^\dagger \tilde{\boldsymbol{\alpha}}_0 - \tilde{\boldsymbol{\alpha}}_r^\dagger \tilde{\boldsymbol{\alpha}}_0^\dagger)\}. \tag{2.3}$$

If $\tilde{\mathscr{H}}_+$ is defined to be the 2^m-dimensional subspace of $\tilde{\mathscr{H}}$ which is spanned by the orthonormal set of 2^m kets

$$2^{-1/2}(|0\ n_1\ n_2 \ldots n_m\rangle + |1\ n_1\ n_2 \ldots n_m\rangle), \tag{2.4a}$$

it is easily verified that with the mapping of $\mathscr{H}$ into $\tilde{\mathscr{H}}_+$, where the basis vector $|n_1\ n_2 \ldots n_m\rangle$ in $\mathscr{H}$ corresponds to the basis vector (2.4a) in $\tilde{\mathscr{H}}_+$ as its image, the operator $\tilde{\mathbf{H}}$ acts in $\tilde{\mathscr{H}}_+$ just as $\mathbf{H}$ does in $\mathscr{H}$. This is seen with the help of table 1 which shows how the operators in the right-hand sides of equation (2.2) act on the basis

† We mark several items in this paper with a tilde to indicate that they are more closely related to the 2^{m+1}-dimensional Hilbert space $\tilde{\mathscr{H}}$ than to the 2^m-dimensional Hilbert space $\mathscr{H}$. For example, the tilde in $\tilde{\boldsymbol{\alpha}}_r$ indicates that this operator acts in $\tilde{\mathscr{H}}$ and not in $\mathscr{H}$.

Table 1. The action of the operators in the right-hand sides of equation (2.2) on the basis vectors of $\tilde{\mathscr{H}}$ ($r = 1, 2, \ldots, m$; $n_r = 0, 1$; $k \equiv n_1 + n_2 + \ldots + n_{r-1}$).

	$\lvert 0\ n_1\ n_2 \ldots n_r = 0 \ldots n_m\rangle$	$\lvert 1\ n_1\ n_2 \ldots n_r = 0 \ldots n_m\rangle$	$\lvert 0\ n_1\ n_2 \ldots n_r = 1 \ldots n_m\rangle$	$\lvert 1\ n_1\ n_2 \ldots n_r = 1 \ldots n_m\rangle$
$\tilde{\boldsymbol{\alpha}}_0^\dagger \tilde{\boldsymbol{\alpha}}_r - \tilde{\boldsymbol{\alpha}}_0 \tilde{\boldsymbol{\alpha}}_r$	$\lvert\text{zero}\rangle$	$\lvert\text{zero}\rangle$	$(-1)^k \lvert 1\ n_1\ n_2 \ldots n_r = 0 \ldots n_m\rangle$	$(-1)^k \lvert 0\ n_1\ n_2 \ldots n_r = 0 \ldots n_m\rangle$
$\tilde{\boldsymbol{\alpha}}_r^\dagger \tilde{\boldsymbol{\alpha}}_0 - \tilde{\boldsymbol{\alpha}}_r^\dagger \tilde{\boldsymbol{\alpha}}_0^\dagger$	$(-1)^k \lvert 1\ n_1 n_2 \ldots n_r = 1 \ldots n_m\rangle$	$(-1)^k \lvert 0\ n_1\ n_2 \ldots n_r = 1 \ldots n_m\rangle$	$\lvert\text{zero}\rangle$	$\lvert\text{zero}\rangle$

kets of $\tilde{\mathcal{H}}$. We can immediately compare the operations ($r = 1, 2, \ldots, m$; $k \equiv n_1 + n_2 + \ldots + n_{r-1}$):

$$\boldsymbol{\alpha}_r|n_1\ n_2 \ldots n_r = 0 \ldots n_m\rangle = |\text{zero}\rangle$$

$$(\tilde{\boldsymbol{\alpha}}_0^\dagger\tilde{\boldsymbol{\alpha}}_r - \tilde{\boldsymbol{\alpha}}_0\tilde{\boldsymbol{\alpha}}_r)(|0\ n_1\ n_2 \ldots n_r = 0 \ldots n_m\rangle + |1\ n_1\ n_2 \ldots n_r = 0 \ldots n_m\rangle) = |\text{zero}\rangle$$

and (2.5)

$$\boldsymbol{\alpha}_r|n_1\ n_2 \ldots n_r = 1 \ldots n_m\rangle = (-1)^k|n_1\ n_2 \ldots n_r = 0 \ldots n_m\rangle$$

$$(\tilde{\boldsymbol{\alpha}}_0^\dagger\tilde{\boldsymbol{\alpha}}_r - \tilde{\boldsymbol{\alpha}}_0\tilde{\boldsymbol{\alpha}}_r)(|0\ n_1\ n_2 \ldots n_r = 1 \ldots n_m\rangle + |1\ n_1\ n_2 \ldots n_r = 1 \ldots n_m\rangle)$$
$$= (-1)^k(|0\ n_1\ n_2 \ldots n_r = 0 \ldots n_m\rangle + |1\ n_1\ n_2 \ldots n_r = 0 \ldots n_m\rangle),$$

and compare the analogous operations of $\boldsymbol{\alpha}_r^\dagger$ and $\tilde{\boldsymbol{\alpha}}_r^\dagger\tilde{\boldsymbol{\alpha}}_0 - \tilde{\boldsymbol{\alpha}}_r^\dagger\tilde{\boldsymbol{\alpha}}_0^\dagger$. (It is trivial to show that with the mapping under consideration the quadratic terms of equation (1.1) act in $\mathcal{H}$ just like the corresponding terms of equation (2.3) act in $\tilde{\mathcal{H}}_+$.) In a similar way we can prove that (again with a suitable mapping) $\tilde{\mathbf{H}}$ acts in the subspace $\tilde{\mathcal{H}}_-$ of $\tilde{\mathcal{H}}$, spanned by the orthonormal set of 2^m kets:

$$2^{-1/2}(|0\ n_1\ n_2 \ldots n_m\rangle - |1\ n_1\ n_2 \ldots n_m\rangle), \tag{2.4b}$$

just like $\mathbf{H}_-$ does in $\mathcal{H}$, if the operator $\mathbf{H}_-$ is constructed from $\mathbf{H}$ (equation (1.1)) by providing the M_r and M_r^* with a minus sign:

$$\mathbf{H}_- \equiv \sum_{r',r=1}^{m}\{\boldsymbol{\alpha}_{r'}^\dagger D_{1r'r}\boldsymbol{\alpha}_r + \boldsymbol{\alpha}_{r'}^\dagger D_{2r'r}\boldsymbol{\alpha}_r^\dagger + \boldsymbol{\alpha}_{r'}D_{3r'r}\boldsymbol{\alpha}_r + \boldsymbol{\alpha}_{r'}D_{4r'r}\boldsymbol{\alpha}_r^\dagger\} - \sum_{r=1}^{m}\{M_r\boldsymbol{\alpha}_r + M_r^*\boldsymbol{\alpha}_r^\dagger\}. \tag{2.6}$$

Since the anticommutation relations for fermion operators are not affected by the simultaneous multiplication of all $\boldsymbol{\alpha}_r$ (and $\boldsymbol{\alpha}_r^\dagger$) by a phase factor $\exp(i\pi)(= \exp(-i\pi)) = -1$, the operators $\mathbf{H}$ and $\mathbf{H}_-$ have the same spectrum. In view of the fact that the Hilbert space $\tilde{\mathcal{H}}$ is the direct sum of the (orthogonal) subspaces $\tilde{\mathcal{H}}_+$ and $\tilde{\mathcal{H}}_-$, we conclude that each level of the spectrum of $\tilde{\mathbf{H}}$ defined in $\tilde{\mathcal{H}}$ has a degeneracy which is twice its degeneracy in the spectrum of $\mathbf{H}$ defined in $\mathcal{H}$. If the spectrum of this $\mathbf{H}$ is characterised by m mode energies (which will be shown presently), then it is evident that the extra degeneracy of the spectrum of $\tilde{\mathbf{H}}$ can be described by an extra mode energy zero so that the spectrum of $\tilde{\mathbf{H}}$ then is characterised by $m + 1$ mode energies. One of these is zero, whereas the other m are given by the mode energies of the spectrum of $\mathbf{H}$.

The diagonalisation of the homogeneous quadratic Hamiltonian $\tilde{\mathbf{H}}$ is standard (see Appendix A) and will be carried out below. The spectrum of such an $\tilde{\mathbf{H}}$ is characterised by $m + 1$ mode energies and because of the even degeneracy just shown of all energy levels, at least one of these mode energies vanishes (one can argue for example that only a zero mode energy allows one to go from one ground state to another). So we can conclude that the spectrum of $\mathbf{H}$ is indeed characterised by m mode energies.

Now we turn to the diagonalisation of $\tilde{\mathbf{H}}$. Following the procedure described in Appendix A, we rewrite equation (2.3) according to equation (A.5) ($\tilde{D}_i$ ($i = 1, 2, 3, 4$) are $(m + 1)$-square matrices):

$$\tilde{\mathbf{H}} \equiv \sum_{r',r=0}^{m}\{\tilde{\boldsymbol{\alpha}}_{r'}^\dagger\tilde{D}_{1r'r}\tilde{\boldsymbol{\alpha}}_r + \tilde{\boldsymbol{\alpha}}_{r'}^\dagger\tilde{D}_{2r'r}\tilde{\boldsymbol{\alpha}}_r^\dagger + \tilde{\boldsymbol{\alpha}}_{r'}\tilde{D}_{3r'r}\tilde{\boldsymbol{\alpha}}_r + \tilde{\boldsymbol{\alpha}}_{r'}\tilde{D}_{4r'r}\tilde{\boldsymbol{\alpha}}_r^\dagger\} \equiv \tilde{\boldsymbol{\alpha}}^\dagger\tilde{\mathcal{D}}\tilde{\boldsymbol{\alpha}}, \tag{2.7}$$

where $\tilde{\boldsymbol{\alpha}}^\dagger$ is a row $2(m + 1)$-vector of operators $\tilde{\boldsymbol{\alpha}}$:

$$\tilde{\boldsymbol{\alpha}}^\dagger \equiv (\tilde{\boldsymbol{\alpha}}_0^\dagger\tilde{\boldsymbol{\alpha}}_1^\dagger\tilde{\boldsymbol{\alpha}}_2^\dagger \ldots \tilde{\boldsymbol{\alpha}}_m^\dagger \quad \tilde{\boldsymbol{\alpha}}_0\tilde{\boldsymbol{\alpha}}_1\tilde{\boldsymbol{\alpha}}_2 \ldots \tilde{\boldsymbol{\alpha}}_m), \tag{2.8}$$

and $\tilde{a}$ the Hermitian-conjugate column vector. The grand-dynamical (Hermitian) matrix $\tilde{\mathscr{D}}$ of the Hamiltonian (2.7) is given by (A and B are m-square matrices, $\tilde{A} \equiv \tilde{D}_1 = -\tilde{D}_4^*$ and $\tilde{B} \equiv \tilde{D}_2 = -\tilde{D}_3^*$ are $(m+1)$-square matrices):

$$\tilde{\mathscr{D}} \equiv \begin{pmatrix} 0 & \frac{1}{2}M_1 & \frac{1}{2}M_2 \ldots & \frac{1}{2}M_m & 0 & \frac{1}{2}M_1^* & \frac{1}{2}M_2^* \ldots & \frac{1}{2}M_m^* \\ \frac{1}{2}M_1^* & & & & -\frac{1}{2}M_1^* & & & \\ \frac{1}{2}M_2^* & & A & & -\frac{1}{2}M_2^* & & B & \\ \ldots & & & & \ldots & & & \\ \frac{1}{2}M_m^* & & & & -\frac{1}{2}M_m^* & & & \\ & & & & & & & \\ 0 & -\frac{1}{2}M_1 & -\frac{1}{2}M_2 \ldots & -\frac{1}{2}M_m & 0 & -\frac{1}{2}M_1^* & -\frac{1}{2}M_2^* \ldots & -\frac{1}{2}M_m^* \\ \frac{1}{2}M_1 & & & & -\frac{1}{2}M_1 & & & \\ \frac{1}{2}M_2 & & -B^* & & -\frac{1}{2}M_2 & & -A^* & \\ \ldots & & & & \ldots & & & \\ \frac{1}{2}M_m & & & & -\frac{1}{2}M_m & & & \end{pmatrix} \equiv \begin{pmatrix} \tilde{A} & \tilde{B} \\ -\tilde{B}^* & -\tilde{A}^* \end{pmatrix} \tag{2.9}$$

The diagonalisation of $\tilde{\mathbf{H}}$ is now performed according to the scheme (cf equation (A.8)):

$$\tilde{\mathbf{H}} \equiv \tilde{a}^\dagger \tilde{\mathscr{D}} \tilde{a} = \tilde{a}^\dagger \tilde{\mathscr{T}}^\dagger \tilde{\mathscr{T}} \tilde{\mathscr{D}} \tilde{\mathscr{T}}^\dagger \tilde{\mathscr{T}} \tilde{a} = \tilde{c}^\dagger \tilde{\mathscr{E}} \tilde{c}, \tag{2.10}$$

where (cf equation (A.6))

$$\tilde{a}^\dagger \tilde{\mathscr{T}}^\dagger = \tilde{c} \equiv (\tilde{\gamma}_0^\dagger \tilde{\gamma}_1^\dagger \tilde{\gamma}_2^\dagger \ldots \tilde{\gamma}_m^\dagger \quad \tilde{\gamma}_0 \tilde{\gamma}_1 \tilde{\gamma}_2 \ldots \tilde{\gamma}_m), \qquad \tilde{\mathscr{T}}^\dagger \equiv \begin{pmatrix} \tilde{U} & \tilde{V}^* \\ \tilde{V} & \tilde{U}^* \end{pmatrix} \tag{2.11}$$

is a row vector of new fermion construction operators $\tilde{\gamma}$ ($\tilde{c}$ the Hermitian-conjugate column vector) and where the unitary matrix $\tilde{\mathscr{T}}^\dagger$ (unitary in order that the $\tilde{\gamma}$ constitute a set of fermion construction operators provided the $\tilde{a}$ do too, see Appendix A) of the partitioned form shown in equation (2.11) (cf equation (A.7)), is chosen so that $\tilde{\mathscr{E}}$ is diagonal and of the form:

$$\tilde{\mathscr{T}} \tilde{\mathscr{D}} \tilde{\mathscr{T}}^\dagger = \tilde{\mathscr{E}} \equiv \operatorname{diag}(\lambda_0, \lambda_1, \lambda_2, \ldots, \lambda_m, -\lambda_0, -\lambda_1, -\lambda_2, \ldots, -\lambda_m). \tag{2.12}$$

(That such a $\tilde{\mathscr{T}}^\dagger$ exists, is proved in Appendix A.) This diagonalisation results in the desired form:

$$\tilde{\mathbf{H}} = \sum_{r=0}^{m} \lambda_r (\tilde{\gamma}_r^\dagger \tilde{\gamma}_r - \tilde{\gamma}_r \tilde{\gamma}_r^\dagger) = \sum_{r=1}^{m} 2\lambda_r \tilde{\gamma}_r^\dagger \tilde{\gamma}_r - \sum_{r=1}^{m} \lambda_r \equiv \sum_{r=1}^{m} \hbar\omega_r (\tilde{\gamma}_r^\dagger \tilde{\gamma}_r - \tfrac{1}{2}). \tag{2.13}$$

(Since we saw above that at least one of the λ_r vanishes†, it is natural to put the columns of $\tilde{\mathscr{T}}^\dagger$ in equation (2.12) in such an order that $\lambda_0 = 0$‡.)

† We can also see this directly: one verifies immediately that the $2(m+1)$-vector $(100 \ldots 0\ 100 \ldots 0)'$ (the prime indicates a column vector) is an eigenvector of $\tilde{\mathscr{D}}$ with vanishing eigenvalue. It can be proved (cf Appendix A) that the multiplicity of a zero eigenvalue of a Hermitian matrix is even if the matrix has the partitioned form of the extreme right-hand side of equation (2.9).

‡ It is not important for our considerations which transformation is actually used in the diagonalisation. However, we want to point out here that in general there is no unique natural choice for the 1st and $(m+2)$-th column of $\tilde{\mathscr{T}}^\dagger$. See Appendix C for a full treatment of this matter.

In view of the connection, discussed in the first part of this section, between the spectra of $\tilde{\mathbf{H}}$ (equation (2.3)) and $\mathbf{H}$ (equation (1.1)), the *spectrum* of $\mathbf{H}$ coincides with that of any operator, also defined in the 2^m-dimensional Hilbert space $\mathscr{H}$, of the form of the extreme right-hand side of equation (2.13) (without tildes) with the values of the $\hbar\omega_r$ unaltered and the $\boldsymbol{\gamma}$ constituting an arbitrary set of fermion construction operators (defined in $\mathscr{H}$). Now one easily shows the existence of a set of fermion construction operators $\boldsymbol{\gamma}$ (which can be defined by their action on 2^m orthonormal eigenkets of the Hamiltonian (1.1)), in terms of which the Hamiltonian (1.1) really (i.e. eigenvalues *and corresponding eigenkets* are the same) can be written in the form:

$$\mathbf{H} = \sum_{r=1}^{m} \hbar\omega_r(\boldsymbol{\gamma}_r^{\dagger}\boldsymbol{\gamma}_r - \tfrac{1}{2}) \tag{2.13'}$$

with the same values of the mode energies $\hbar\omega_r$ as in equation (2.13). Note that the fermion construction operators $\tilde{\boldsymbol{\gamma}}$ and $\boldsymbol{\gamma}$ in equations (2.13) and (2.13') are different operators since they are defined in different Hilbert spaces. The direct connection between the $\boldsymbol{\gamma}$ in equation (2.13') and the $\boldsymbol{\alpha}$ in equation (1.1) in general is very complicated and will be discussed in § 4.

In conclusion, the eigenvalues of the $2(m+1)$-square Hermitian matrix (2.9) can be identified with (half) the mode energies $\hbar\omega_r$ of the spectrum of the Hamiltonian (1.1) or (2.13'). To be more specific: two zero eigenvalues are not relevant and to be excluded; one finds for each $r = 1, 2, \ldots, m$ the values $\frac{1}{2}\hbar\omega_r$ and $-\frac{1}{2}\hbar\omega_r$ among the remaining eigenvalues. Note that one is free to choose for each r the sign of $\hbar\omega_r$ and that this choice has no influence on the spectrum one derives from equation (2.13') (cf the last footnote in Appendix A). If one chooses all mode energies $\hbar\omega_r \geqslant 0$, equation (2.13') immediately yields the ground-state energy of the Hamiltonian $\mathbf{H}$: the lowest eigenvalue of $\mathbf{H}$ then equals minus half times the sum of all these mode energies.

3. Simplification in case the grand-dynamical matrix (2.9) is real

In many practical cases tricks can be applied to simplify the calculation. In this section we consider the situation that all coefficients in the Hamiltonian (1.1) are real; it is then possible to carry out a reduction of the $2(m+1)$-square grand-dynamical matrix (2.9) to an m-square real symmetric matrix of which the eigenvalues are also directly related to the mode energies. This is reached by using Appendix A of the paper by Lieb *et al* (1961), where a general method has been given for the diagonalisation of a homogeneous quadratic form in fermion construction operators *in case all coefficients are real.* From the treatment of Lieb *et al* we conclude that the mode energies which according to § 2 appear as eigenvalues of $2\tilde{\mathscr{D}}$, are also found as the square roots of the eigenvalues of 4 times the real symmetric matrix

$$\tilde{D} \equiv (\tilde{A} - \tilde{B})(\tilde{A} + \tilde{B}) =$$

$$\begin{pmatrix} 0 & 0 & 0 & \ldots & 0 \\ M_1 & & & & \\ M_2 & & A-B & & \\ \ldots & & & & \\ M_m & & & & \end{pmatrix} \begin{pmatrix} 0 & M_1 & M_2 & \ldots & M_m \\ 0 & & & & \\ 0 & & A+B & & \\ \ldots & & & & \\ 0 & & & & \end{pmatrix} = \begin{pmatrix} 0 & 0 & 0 & \ldots & 0 \\ 0 & & & & \\ 0 & & D & & \\ \ldots & & & & \\ 0 & & & & \end{pmatrix}, \tag{3.1}$$

where equation (2.9) has been used in order to evaluate the matrices and where the real

symmetric matrix D has been defined by its elements:

$$D_{ij} = [(A-B)(A+B)]_{ij} + M_i M_j. \tag{3.2}$$

Because it is natural to identify the apparent zero eigenvalue of the matrix in the right-hand side of equation (3.1) with the redundant eigenvalue which was introduced in § 2 by transferring our considerations to the larger Hilbert space $\tilde{\mathscr{H}}$, we conclude immediately that the eigenvalues of the matrix $4D$ represent the squares of the mode energies which characterise the spectrum of the Hamiltonian (1.1) (*in case all coefficients are real*!). According to the last paragraph of § 2 the ground-state energy of the Hamiltonian is given by minus half times the sum of the mode energies provided these are taken as non-negative.

We take as an example a fermion Hamiltonian of the form (1.3) or, adding a constant, of the form:

$$\mathbf{H} \equiv \sum_{r=1}^{m} \mathbf{H}_r \equiv \sum_{r=1}^{m} \{\lambda_r(\boldsymbol{\alpha}_r^\dagger \boldsymbol{\alpha}_r - \boldsymbol{\alpha}_r \boldsymbol{\alpha}_r^\dagger) + \mu_r \boldsymbol{\alpha}_r + \mu_r^* \boldsymbol{\alpha}_r^\dagger\}, \qquad \begin{matrix}\lambda_r \text{ real numbers,} \\ \mu_r \text{ complex numbers}\end{matrix} \tag{3.3}$$

(this form can always be obtained for a Hamiltonian (1.1) by diagonalisation of the homogeneous quadratic part; in practice, however, the complete diagonalisation would then require two matrix diagonalisations, and it seems preferable to apply the single diagonalisation of $\tilde{\mathscr{D}}$ given by equation (2.9) for finding the mode energies). We first remark that the spectrum of the Hamiltonian (3.3) is not changed if we replace the coefficients μ_r by their absolute values since the anticommutation relations for fermion operators are not affected by the simultaneous multiplication of all $\boldsymbol{\alpha}_r$ and $\boldsymbol{\alpha}_r^\dagger$ by a phase factor $\exp(\mathrm{i}\phi_r)$ and $\exp(-\mathrm{i}\phi_r)$, respectively (ϕ_r real). Then we obtain for the matrix D according to equation (3.2):

$$D \equiv \begin{pmatrix} \lambda_1^2 + |\mu_1|^2 & |\mu_1\mu_2| & \cdots & |\mu_1\mu_m| \\ |\mu_2\mu_1| & \lambda_2^2 + |\mu_2|^2 & \cdots & |\mu_2\mu_m| \\ \cdots & \cdots & \cdots & \cdots \\ |\mu_m\mu_1| & |\mu_m\mu_2| & \cdots & \lambda_m^2 + |\mu_m|^2 \end{pmatrix}. \tag{3.4}$$

As argued above the eigenvalues of $4D$ represent the squares of the mode energies of the Hamiltonian (3.3). The ground-state energy of this Hamiltonian equals minus the sum of the (non-negative) square roots of the eigenvalues of D.

Note that all m values of λ_r and of μ_r make themselves felt in the value of each particular mode energy just as we expected in § 1 in connection with our comparison of the fermion and boson situation.

4. Discussion

We have seen that the formalisms of boson and fermion construction operators both have the important property that an m-mode quadratic Hamiltonian with a linear part immediately can be associated with a spectrum characterised by m mode energies.

The essential point in which the treatment for fermions as given in this paper differs from the familiar treatment for bosons is, that the 'transforming away' of the linear part in the boson case is performed by a simple 'translation' transformation of the form (1.4)

of the construction operators, whereas in the fermion case we homogenised the Hamiltonian (1.1) by the introduction of a ghost particle (§ 2).

In this section we want to prove that without such a trick a linear transformation applied to the fermion construction operators cannot lead to the desired result. To this end we consider the fermion construction operators $\boldsymbol{\gamma}$ in terms of which the Hamiltonian (1.1) can be written in the form (2.13′). According to § 2 such $\boldsymbol{\gamma}$ exist. Of course it is not surprising that the 2^m-square matrices by which each of these construction operators $\boldsymbol{\gamma}$ can be represented, in one way or another are expressible in the matrices corresponding to the operators $\boldsymbol{\alpha}$ occurring in equation (1.1). In the following two examples such expressions relating $\boldsymbol{\gamma}$ and $\boldsymbol{\alpha}$ are easily written down. We shall see that in these examples the expressions are much more complicated than merely linear, which would be necessary to solve the diagonalisation problem by means of a linear transformation without an additional trick.

Example 1. It is quite easy to treat the case of a two-dimensional Hilbert space in which the one-mode Hamiltonian is given as:

$$\mathbf{H} \equiv 2\lambda \boldsymbol{\alpha}^{\dagger}\boldsymbol{\alpha} + \mu\boldsymbol{\alpha} + \mu^{*}\boldsymbol{\alpha}^{\dagger}, \qquad \lambda \text{ real number, } \mu \text{ non-zero complex number,} \tag{4.1}$$

and to find a construction-operator pair $\boldsymbol{\gamma}$, $\boldsymbol{\gamma}^{\dagger}$ so that the Hamiltonian can be rewritten as (mode energy and ground-state energy follow from the treatment of the Hamiltonian (3.3) with $m = 1$):

$$\mathbf{H} = 2(\lambda^2 + |\mu|^2)^{1/2}\boldsymbol{\gamma}^{\dagger}\boldsymbol{\gamma} + \lambda - (\lambda^2 + |\mu|^2)^{1/2}. \tag{4.2}$$

One can simply work in a representation where the $\boldsymbol{\alpha}$-operators are represented by:

$$\boldsymbol{\alpha} \equiv \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \qquad \boldsymbol{\alpha}^{\dagger} \equiv \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}, \qquad 1 - 2\boldsymbol{\alpha}^{\dagger}\boldsymbol{\alpha} \equiv \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \tag{4.3}$$

and find after a somewhat tedious algebraic calculation that one can take $\boldsymbol{\gamma}$ as:

$$\boldsymbol{\gamma} = \tfrac{1}{2}(\lambda^2 + |\mu|^2)^{-1/2}\{[(\lambda^2 + |\mu|^2)^{1/2} + \lambda]\boldsymbol{\alpha} - [(\lambda^2 + |\mu|^2)^{1/2} + \lambda]^{-1}\mu^{*2}\boldsymbol{\alpha}^{\dagger} + \mu^{*}(1 - 2\boldsymbol{\alpha}^{\dagger}\boldsymbol{\alpha})\}. \tag{4.4}$$

Note that the transformation (4.4) is not a linear one. Note further that even in case the Hamiltonian (4.1) is purely linear ($\lambda = 0$), it is by equation (4.2) rewritten as a quadratic expression in construction operators in accordance with the trivial fact that the spectrum is characterised by one mode energy (cf the situation in the boson case where $\lambda = 0$ prevents one from using equation (1.4) for transforming the linear Hamiltonian into a quadratic one).

Example 2. Consider the (non-zero) linear Hamiltonian

$$\mathbf{H} \equiv \sum_{r=1}^{m} (\mu_r \boldsymbol{\alpha}_r + \mu_r^{*}\boldsymbol{\alpha}_r^{\dagger}), \qquad \mu_r \text{ complex numbers,} \tag{4.5}$$

defined in a 2^m-dimensional Hilbert space. It is easily verified that the operator

$$\boldsymbol{\beta}_1 = C^{-1}\sum_{r=1}^{m} \mu_r \boldsymbol{\alpha}_r, \qquad C \equiv \Big(\sum_{r=1}^{m} |\mu_r|^2\Big)^{1/2} \tag{4.6}$$

satisfies the anticommutation relation $[\boldsymbol{\beta}_1, \boldsymbol{\beta}_1^{\dagger}]_+ = 1$ and therefore can be considered as

the first fermion construction operator out of a set of m. By the corresponding transformation the Hamiltonian is changed into:

$$\mathbf{H} = C(\boldsymbol{\beta}_1 + \boldsymbol{\beta}_1^\dagger). \tag{4.7}$$

Using the transformation (4.4) (read $\boldsymbol{\gamma}_1$ and $\boldsymbol{\beta}_1$ instead of $\boldsymbol{\gamma}$ and $\boldsymbol{\alpha}$, respectively) for the case $\lambda = 0$ and μ (which now equals C) positive:

$$\boldsymbol{\gamma}_1 = \tfrac{1}{2}\boldsymbol{\beta}_1 - \tfrac{1}{2}\boldsymbol{\beta}_1^\dagger + \tfrac{1}{2}(1 - 2\boldsymbol{\beta}_1^\dagger\boldsymbol{\beta}_1), \tag{4.8}$$

we obtain according to equation (4.2)

$$\mathbf{H} = 2C\boldsymbol{\gamma}_1^\dagger\boldsymbol{\gamma}_1 - C. \tag{4.9}$$

With this we have found that one mode energy equals $2C$, the $m-1$ remaining ones obviously being zero.

In this example the transformation of the $\boldsymbol{\alpha}$ into $\boldsymbol{\gamma}_1$ is extremely complicated and certainly not a linear one. This is seen from equations (4.6) and (4.8) which yield:

$$\boldsymbol{\gamma}_1 = \tfrac{1}{2}C^{-1}\sum_{r=1}^{m}\mu_r\boldsymbol{\alpha}_r - \tfrac{1}{2}C^{-1}\sum_{r=1}^{m}\mu_r^*\boldsymbol{\alpha}_r^\dagger + \tfrac{1}{2}(1 - 2C^{-2}\sum_{r',r=1}^{m}\mu_{r'}^*\mu_r\boldsymbol{\alpha}_{r'}^\dagger\boldsymbol{\alpha}_r). \tag{4.10}$$

With these two examples we hope to have convinced the reader that in general we can only carry out the diagonalisation of quadratic Hamiltonians with a linear part by a *linear* transformation of construction operators if we call in the aid of an extra construction-operator pair $\tilde{\boldsymbol{\alpha}}_0, \tilde{\boldsymbol{\alpha}}_0^\dagger$, in the way we did in § 2. Our results show that without incorporating such an auxiliary $\tilde{\boldsymbol{\alpha}}_0$ into the problem, in general the question of the transformation does not fit in a natural way into the formalism of fermion construction operators.

5. Conclusion

For boson construction operators it is well known that a linear part in a quadratic m-mode Hamiltonian of the form (1.1) is easily transformed away by a 'translation' transformation of the form (1.4). The fact that many problems in terms of construction operators allow parallel treatments for the boson and fermion case, strongly suggests that in the fermion case the spectrum is also characterised by m mode energies (i.e. the energy eigenvalues are given by an equation of the form (1.7), $n_r = 0$ or 1) and that in this case as well a linear part does not present difficulties. We could indeed show the spectrum to have this property, but it emerges that there is no question of solving the fermion problem by considering it as the counterpart of the corresponding boson problem.

The formalism of the fermion construction operators allows a relatively simple calculation of the spectrum. We succeeded (§ 2) in establishing the $2(m+1)$-square Hermitian matrix $\tilde{\mathscr{D}}$ (equation (2.9); the m-square matrices A and B are defined by equation (2.1)), the eigenvalues of which equal (half times) the mode energies. In case all coefficients in the Hamiltonian are real (§ 3), we may even find these energies by diagonalising a real symmetric matrix D of order only m, the elements of which are given by equation (3.2). Each of these matrices $\tilde{\mathscr{D}}$ and D contain the same information about the spectrum as the (in general much larger) matrices of order 2^m like equation (1.9), which one would use when calculating the spectrum by a brute-force technique; in

addition the construction of the last kind of matrix is in practice more complicated. The ground-state energy of the Hamiltonian (1.1) can be found from the mode energies according to the considerations in the last paragraph of § 2.

We recognised the possibility of writing down the Hamiltonian (1.1) in the form (2.13′). In contrast with the boson case (cf equation (1.4)) this does not follow from the application of a simple linear transformation to the construction operators, which accomplishes this diagonalisation: in the fermion case such a transformation in general does not exist (§ 4). Rather is the form (2.13′) an immediate consequence of the property of the spectrum to be characterised by m mode energies. For the same reason a purely linear fermion Hamiltonian can also be written into the homogeneous quadratic form (2.13′) as we showed explicitly in § 4 (example 2).

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Appendix A. Diagonalisation of the general homogeneous quadratic fermion Hamiltonian

In this appendix we consider the diagonalisation of a Hamiltonian of the general form (m denotes an arbitrary positive integer):

$$\mathbf{H} \equiv \sum_{r',r=1}^{m} (\boldsymbol{\alpha}_{r'}^{\dagger} D_{1r'r} \boldsymbol{\alpha}_r + \boldsymbol{\alpha}_{r'}^{\dagger} D_{2r'r} \boldsymbol{\alpha}_r^{\dagger} + \boldsymbol{\alpha}_{r'} D_{3r'r} \boldsymbol{\alpha}_r + \boldsymbol{\alpha}_{r'} D_{4r'r} \boldsymbol{\alpha}_r^{\dagger}), \tag{A.1}$$

where the $\boldsymbol{\alpha}_r$, $\boldsymbol{\alpha}_r^{\dagger}$ constitute a set of m fermion-operator pairs and where the coefficients $D_{ir'r}$ ($i = 1, 2, 3, 4$) can be complex numbers. The treatment, which is a direct translation of the treatment of the analogous problem in the boson case in C § 4, is more general than the one of Lieb *et al* (1961) who assumed the coefficients to be real. The approach of Lieb *et al* requires an orthogonal diagonalisation of a (real) symmetric matrix of order m, whereas our approach involves the unitary diagonalisation of a Hermitian matrix of order $2m$.

An operator of the form (A.1) is Hermitian if and only if the following relations hold:

$$\begin{aligned} &D_{1r'r} - D_{4rr'} = D_{1rr'}^{*} - D_{4r'r}^{*}, \qquad && D_{1rr} = D_{1rr}^{*}, \\ &D_{2r'r} - D_{2rr'} = D_{3rr'}^{*} - D_{3r'r}^{*}, && 1 \leqslant r', r \leqslant m. \end{aligned} \tag{A.2}$$

(Note: the first line of this equation implies that the diagonal elements of D_1 and D_4 are real.) For the subsequent analysis it is essential that

$$\begin{aligned} &D_{1r'r} = D_{1rr'}^{*} = -D_{4rr'}, \qquad && D_{2r'r} = -D_{2rr'} = D_{3rr'}^{*}, \\ &D_{3r'r} = -D_{3rr'} = D_{2rr'}^{*}, && D_{4r'r} = D_{4rr'}^{*} = -D_{1rr'}, \end{aligned} \qquad 1 \leqslant r', r \leqslant m, \tag{A.3}$$

which obviously can be assumed without restricting the generality: a rewriting in this sense modifies the (Hermitian) expression (A.1) at most by an additive (real) constant.

Then the $2m$-square matrix†

$$\mathscr{D} \equiv \begin{pmatrix} D_1 & D_2 \\ D_3 & D_4 \end{pmatrix} \equiv \begin{pmatrix} A & B \\ -B^* & -A^* \end{pmatrix} \tag{A.4}$$

has the form indicated and is Hermitian (which implies that A is Hermitian and B skew-symmetric). As in C we call $\mathscr{D}$ the grand-dynamical matrix of the Hamiltonian (A.1) and use it to rewrite equation (A.1) in matrix notation:

$$\mathbf{H} \equiv \boldsymbol{a}^\dagger \mathscr{D} \boldsymbol{a}, \qquad \boldsymbol{a}^\dagger \equiv (\boldsymbol{\alpha}^\dagger \ \boldsymbol{\alpha}), \qquad \boldsymbol{a} \equiv \begin{pmatrix} \boldsymbol{\alpha} \\ \boldsymbol{\alpha}^\dagger \end{pmatrix}, \tag{A.5}$$

where $\boldsymbol{a}^\dagger$ and $\boldsymbol{a}$ are a row and column vector, respectively, each with $2m$ fermion construction operators as elements, and where $\boldsymbol{a}^\dagger$ and $\boldsymbol{a}$ are m-vectors (no confusion is to be expected because no extra symbols indicate that $\boldsymbol{\alpha}^\dagger$ and $\boldsymbol{\alpha}$ in $\boldsymbol{a}^\dagger$ are row m-vectors and in $\boldsymbol{a}$ column m-vectors). Taking into account that in a transformation to new construction operators $\boldsymbol{\gamma}$ of the form:

$$\boldsymbol{c} = \mathscr{T} \boldsymbol{a} \qquad \text{or} \qquad \begin{pmatrix} \boldsymbol{\gamma} \\ \boldsymbol{\gamma}^\dagger \end{pmatrix} = \begin{pmatrix} P & Q \\ Q^* & P^* \end{pmatrix} \begin{pmatrix} \boldsymbol{\alpha} \\ \boldsymbol{\alpha}^\dagger \end{pmatrix}, \tag{A.6}$$

the matrix $\mathscr{T}$ has the partitioned square form shown in equation (A.6) and that $\mathscr{T}$ should be unitary in order that the $\boldsymbol{\gamma}$ constitute a set of fermion operators provided the $\boldsymbol{\alpha}$ do as well, we have:

$$\mathscr{T} \equiv \begin{pmatrix} P & Q \\ Q^* & P^* \end{pmatrix}, \qquad \mathscr{T}^{-1} = \mathscr{T}^\dagger = \begin{pmatrix} P^\dagger & (Q^*)^\dagger \\ Q^\dagger & (P^*)^\dagger \end{pmatrix} \equiv \begin{pmatrix} U & V^* \\ V & U^* \end{pmatrix}. \tag{A.7}$$

Now in a diagonalisation according to the scheme

$$\mathbf{H} \equiv \boldsymbol{a}^\dagger \mathscr{D} \boldsymbol{a} = \boldsymbol{a}^\dagger \mathscr{T}^\dagger (\mathscr{T}^\dagger)^{-1} \mathscr{D} \mathscr{T}^{-1} \mathscr{T} \boldsymbol{a} = \boldsymbol{c}^\dagger \mathscr{E} \boldsymbol{c} \tag{A.8}$$

with a matrix $\mathscr{T}$ of the form (A.7), the diagonal matrix $\mathscr{E}$ necessarily has the form:

$$(\mathscr{T}^\dagger)^{-1} \mathscr{D} \mathscr{T}^{-1} = \mathscr{E} \equiv \tfrac{1}{2}\hbar \operatorname{diag}(\omega_1, \omega_2, \ldots, \omega_m, -\omega_1, -\omega_2, \ldots, -\omega_m). \tag{A.9}$$

The right-hand side has the special form indicated, because the matrix $(\mathscr{T}^\dagger)^{-1} \mathscr{D} \mathscr{T}^{-1} = \mathscr{T} \mathscr{D} \mathscr{T}^\dagger$ is Hermitian (so the diagonal elements are real), while the right-lower m-square matrix of a product of the form $(\mathscr{T}^\dagger)^{-1} \mathscr{D} \mathscr{T}^{-1}$ equals minus the complex conjugate of the left-upper m-square matrix of that product, if $\mathscr{D}$ and $\mathscr{T}^{-1}$ have the partitioned forms (A.4) and (A.7), respectively.

We now turn our attention to the construction of a unitary matrix $\mathscr{T}^{-1}$ of the partitioned form (A.7) which diagonalises $\mathscr{D}$ according to equation (A.9). We assume first that $\mathscr{D}$ is non-singular, i.e. $\mathscr{D}$ has no zero eigenvalues. Then half of the eigenvalues of $\mathscr{D}$ are positive, the other half negative; apart from the sign the two halves contain the same eigenvalues. To see this we consider an arbitrary eigenvalue λ with multiplicity n.

† In this appendix (and in this paper) the notation of C is followed throughout. Accordingly matrices are often represented in partitioned form: a $2m$-square matrix is represented by four m-square matrices and $2m$-vectors by two m-vectors. Script letters are used to indicate $2m$-square matrices and $2m$-vectors, Latin or Greek letters are used for m-square matrices and m-vectors. By A^* we denote the complex conjugate of the matrix A (elements: $(A^*)_{r's} = (A_{r's})^*$).

Let $(u_r\ v_r)'$ ($r = 1, 2, \ldots, n$; u_r and v_r are column m-vectors and the prime denotes a column vector) constitute an orthogonal set of n eigenvectors associated with the eigenvalue λ. Then we have:

$$\begin{aligned} Au_r + Bv_r &= \lambda u_r & \qquad Av_r^* + Bu_r^* &= -\lambda v_r^* \\ & \text{or} & & \\ -B^*u_r - A^*v_r &= \lambda v_r & \qquad -B^*v_r^* - A^*u_r^* &= -\lambda u_r^*, \end{aligned} \tag{A.10}$$

so that $(v_r^*\ u_r^*)'$ is an eigenvector associated with the eigenvalue $-\lambda$ if $(u_r\ v_r)'$ is an eigenvector associated with the eigenvalue λ. Since obviously together with the $(u_r\ v_r)'$ also the $(v_r^*\ u_r^*)'$ ($r = 1, 2, \ldots, n$) are perpendicular to each other, we see that the multiplicity of $-\lambda$ is at least that of λ. Starting from eigenvalue $-\lambda$ instead of λ we prove in a similar way that the multiplicity of $-\lambda$ is at most that of λ so that the multiplicities of λ and $-\lambda$ are the same. For the construction of a $\mathcal{T}^{-1}$ with the above-mentioned properties we start from an arbitrary unitary matrix $\mathcal{T}^{-1}$ which diagonalizes $\mathcal{D}$ but which possibly does not have the form (A.7). We only arrange that the *first* m columns $(u_r\ v_r)'$ ($r = 1, 2, \ldots, m$) of $\mathcal{T}^{-1}$ are associated with the *positive* eigenvalues of $\mathcal{D}$. Since the $(u_r\ v_r)'$ are perpendicular to each other, also the $(v_r^*\ u_r^*)'$ constitute an orthogonal set. Furthermore the $(v_r^*\ u_r^*)'$, being associated with the negative eigenvalues of $\mathcal{D}$ (cf equation (A.10)), are perpendicular to the m vectors $(u_r\ v_r)'$ (different eigenvalues). Therefore the matrix arising from the replacement of the last m columns of the chosen $\mathcal{T}^{-1}$ by $(v_1^*\ u_1^*)', (v_2^*\ u_2^*)', \ldots, (v_m^*\ u_m^*)'$, is a unitary matrix with the required properties: it has the form (A.7) and the diagonalisation property (A.9).

Now we concentrate on the case that $\mathcal{D}$ is singular. After the considerations above it is easily verified that the multiplicity of the eigenvalue 0 should be even: $2n$, say. For the construction of a $\mathcal{T}^{-1}$ we obviously only have to show the existence of an orthonormal set $\mathcal{B}$ of eigenvectors of $\mathcal{D}$ associated with the eigenvalue 0, which can serve as columns in a matrix $\mathcal{T}^{-1}$ of the form (A.7):

$$\mathcal{B} \equiv \{(u_1\ v_1)', (u_2\ v_2)', \ldots, (u_n\ v_n)', (v_1^*\ u_1^*)', (v_2^*\ u_2^*)', \ldots, (v_n^*\ u_n^*)'\}. \tag{A.11}$$

The existence of such a set of eigenvectors is guaranteed by the theorem formulated in Appendix B (cf equation (B.6)). This theorem can be proved in principle by adding to the grand-dynamical matrix (A.4) the matrix $x\ \mathrm{diag}(1, 1, \ldots, 1, -1, -1, \ldots, -1)$, with x a small positive number. For the columns of $\mathcal{T}^{-1} \equiv \mathcal{T}^{-1}(x = 0)$ one can take the limits of the columns of $\mathcal{T}^{-1}(x)$ for x tending to zero. In Appendix B another proof of the theorem will be given. This proof simultaneously suggests an algorithm (see the remark at the end of Appendix B†), which enables us to calculate *in practice* $2n$ vectors constituting an orthonormal set $\mathcal{B}$ of the required form (A.11) so that they can serve as columns of a $\mathcal{T}^{-1}$.

To summarise, we have shown that the general homogeneous quadratic fermion Hamiltonian (A.1) (or any other Hermitian operator of that form) can be diagonalised by a homogeneous linear transformation applied to the construction operators. Our treatment shows the way for actually calculating the transformation in practice. The

† For real matrices $\mathcal{D}$ the algorithm, given in Appendix A of the paper of Lieb *et al* (1961), is to be preferred because of the lower order of the matrix to be diagonalised (cf the end of the first paragraph of this appendix).

diagonalised Hamiltonian is obtained by substitution of equations (A.9) and (A.6) into equation (A.8)†:

$$\mathbf{H} = \sum_{r=1}^{m} \hbar\omega_r(\boldsymbol{\gamma}_r^{\dagger}\boldsymbol{\gamma}_r - \tfrac{1}{2}). \tag{A.12}$$

Appendix B

In this appendix we prove a theorem which was applied in Appendix A. The proof needs a lemma (Lemma 2) which in turn needs Lemma 1.

Lemma 1. Let $\mathcal{S}$ be an n-dimensional subspace of the $2m$-dimensional vector space with the property that, if the vector $(r\ s)'$ lies in $\mathcal{S}$, then also the vector $(s^*\ r^*)'$ does. Then there exists an orthogonal basis $\mathcal{B}''$ of $\mathcal{S}$ of the form:

$$\mathcal{B}'' \equiv \{(t_1\ \eta_1 t_1^*)', (t_2\ \eta_2 t_2^*)', \ldots, (t_n\ \eta_n t_n^*)'\}, \tag{B.1}$$

where each η_i $(i = 1, 2, \ldots, n)$ denotes one of the values 1 and -1. In the case that $\mathcal{S}$ is spanned by a set of n linearly independent *real* vectors, the column m-vectors t_i can be chosen to be real.

Proof. To find a first vector of $\mathcal{B}''$, we choose an arbitrary vector $(r\ s)'$ lying in $\mathcal{S}$. By hypothesis also $(s^*\ r^*)'$ lies in $\mathcal{S}$ and consequently the two vectors $(r \pm s^*\ s \pm r^*)'$. Since at least one of these two vectors is non-zero, we have a first vector of $\mathcal{B}''$. Next we find vector by vector n orthogonal vectors which constitute a basis $\mathcal{B}''$ of the form (B.1) by the following procedure. Suppose we have found already an orthogonal set of $k < n$ vectors lying in $\mathcal{S}$ of the form $(t_i\ \eta_i t_i^*)'$ $(i = 1, 2, \ldots, k)$; in what follows we shall call these k vectors the original vectors. Then we choose an arbitrary vector $(r\ s)'$ which lies in $\mathcal{S}$ and which is linearly independent of the k original vectors. We observe that the two vectors $(r \pm s^*\ s \pm r^*)'$ (which also lie in $\mathcal{S}$) cannot simultaneously be linear combinations of the k original vectors (note that also the zero vector is a linear combination of these k vectors). This is true because we would have:

$$\begin{aligned} r + s^* &= a_1 t_1 + a_2 t_2 + \ldots + a_k t_k \\ s + r^* &= a_1\eta_1 t_1^* + a_2\eta_2 t_2^* + \ldots + a_k\eta_k t_k^* \end{aligned} \tag{B.2}$$

and

$$\begin{aligned} r - s^* &= b_1 t_1 + b_2 t_2 + \ldots + b_k t_k \\ s - r^* &= b_1\eta_1 t_1^* + b_2\eta_2 t_2^* + \ldots + b_k\eta_k t_k^*, \end{aligned} \qquad a_i, b_i \text{ complex scalars,}$$

whence

$$\begin{aligned} 2r &= (a_1 + b_1)t_1 + (a_2 + b_2)t_2 + \ldots + (a_k + b_k)t_k \\ 2s &= (a_1 + b_1)\eta_1 t_1^* + (a_2 + b_2)\eta_2 t_2^* + \ldots + (a_k + b_k)\eta_k t_k^*, \end{aligned} \tag{B.3}$$

which contradicts our assumption that $(r\ s)'$ is linearly *in*dependent of the k original vectors. So we have found at least one vector of the form $(t\ \eta t^*)'$ with the property that

† Note that one is free to interchange the r-th and $(m+r)$-th column $(1 \leqslant r \leqslant m)$ of $\mathcal{T}^{-1}$ for an arbitrary number of r's, because this manipulation does not affect the required form (A.7) of $\mathcal{T}^{-1}$. The values of the corresponding $\hbar\omega_r$ in equation (A.12) then turn into their opposites, but from equation (A.12) we easily see that the spectrum remains the same, as it should.

it is linearly independent of the k original vectors. Now the familiar orthogonalisation procedure of Gram–Schmidt turns this $(t\ \eta t^*)'$ into a vector $(t_{k+1}\ \eta t_{k+1}^*)'$ with the same η which is perpendicular to the k original vectors. This is seen by taking into account that the scalar product of $(t\ \eta t^*)'$ by each of the k original vectors $(t_i\ \eta_i t_i^*)'$ is real or purely imaginary (possibly zero) depending on whether η and η_i are equal or not and that any vector of the form $(t\ \eta t^*)'$ is changed into a vector of the form $(t\ -\eta t^*)'$ by multiplication by the scalar i. Thus we see how step by step an orthogonal basis $\mathscr{B}''$ of $\mathscr{S}$ of the form (B.1) can be found. The statement about the case that $\mathscr{S}$ is spanned by a set of n linearly independent real vectors, is trivial (note that the purely imaginary result for a scalar product of two real vectors with different η is necessarily zero).

Lemma 2. Let $\mathscr{D}$ be a $2m$-square Hermitian singular matrix of the partitioned form:

$$\mathscr{D} \equiv \begin{pmatrix} A & B \\ -B^* & -A^* \end{pmatrix}, \tag{B.4}$$

where A and B are m-square matrices. Let furthermore $2n$ be the multiplicity of the eigenvalue 0 of $\mathscr{D}$ and $\mathscr{S}$ the $2n$-dimensional subspace of eigenvectors of $\mathscr{D}$, associated with the eigenvalue 0. Then there exists an orthonormal basis $\mathscr{B}'$ of $\mathscr{S}$ of the form:

$$\mathscr{B}' \equiv \{(t_1\ t_1^*)', (t_2\ t_2^*)', \ldots, (t_n\ t_n^*)', (t_{n+1}\ -t_{n+1}^*)', (t_{n+2}\ -t_{n+2}^*)', \ldots, (t_{2n}\ -t_{2n}^*)'\}. \tag{B.5}$$

In the case that the matrix $\mathscr{D}$ is real, the column m-vectors t_i $(i = 1, 2. \ldots, 2n)$ can be chosen to be real.

Preremark. In Appendix A we saw already that the multiplicity of the eigenvalue 0 of a Hermitian matrix $\mathscr{D}$ of the form (B.4) is even. The proof was based on the fact that according to equation (A.10) the non-zero eigenvalues of $\mathscr{D}$ occur in pairs $\{\lambda, -\lambda\}$ as do the corresponding eigenvectors.

Proof. Reading equation (A.10) with $\lambda = 0$ we see that $\mathscr{S}$ satisfies the condition of Lemma 1 (with $2n$ instead of n). Therefore there exists for $\mathscr{S}$ an orthonormal basis $\mathscr{B}''$ of $2n$ vectors of the form $(t\ \eta t^*)'$ (the vectors of $\mathscr{B}''$ can be normalised by real scalars). From $\mathscr{B}''$ a basis $\mathscr{B}'$ of the form (B.5) is easily constructed because we can change any vector of the form $(t\ \eta t^*)'$ into a vector of the form $(t\ -\eta t^*)'$ by multiplication by the scalar i. The lemma has been proved as far as a general *complex* $\mathscr{D}$ is concerned.

The proof of the statement of the lemma for a *real* $\mathscr{D}$ is somewhat more complicated. We start from an orthonormal basis $\mathscr{B}''$ of $2n$ *real* vectors of the form $(t\ \eta t)'$, which exists according to Lemma 1. Then in $\mathscr{B}''$ exactly n of the η's equal one, the remaining n η's being minus one. To see this we include in our considerations the eigenvectors of $\mathscr{D}$, associated with non-zero eigenvalues. Starting from any normalised real eigenvector $(u\ v)'$ of $\mathscr{D}$, associated with a positive eigenvalue λ, we can construct as follows an orthonormal pair of vectors, each vector of the pair being of the form $(t\ \eta t)'$ but with different η's for the two vectors. Taking into account that $(v\ u)'$ is an eigenvector of $\mathscr{D}$ associated with the eigenvalue $-\lambda$ and that consequently (the eigenvalues λ and $-\lambda$ are different) $(v\ u)'$ is perpendicular to $(u\ v)'$, we easily verify that the vectors $2^{-1/2}(u \pm v\ v \pm u)'$ constitute a pair with the required properties. It is now clear how to construct, starting from an orthonormal set of $m-n$ real eigenvectors $(u\ v)'$ associated with the positive eigenvalues of $\mathscr{D}$, an orthonormal set of $2(m-n)$ vectors, $m-n$ of them being of the form $(t\ t)'$ and the remaining $m-n$ of the form $(t\ -t)'$. All these $2(m-n)$ vectors are orthogonal to (the vectors of) $\mathscr{S}$. Now concentrating on the orthonormal set of $m-n$ vectors of the form $(t\ t)'$ we observe that the number of vectors of the form $(t\ t)'$ in

the $\mathscr{B}''$ obtained above cannot exceed n. This is because we would have more than m perpendicular (real) $2m$-vectors of the form $(t\ t)'$ and consequently more than m perpendicular m-vectors t. In a similar way it is seen that the number of vectors in $\mathscr{B}''$ of the form $(t\ -t)'$ cannot exceed n. So exactly n vectors in the $\mathscr{B}''$ obtained are of the form $(t\ t)'$ and exactly n of the form $(t\ -t)'$. We see that the basis $\mathscr{B}''$ as it presents itself, in fact has already the form (B.5) required for $\mathscr{B}'$, with real vectors t_i. Lemma 2 has been proved completely.

With the help of Lemma 2 we can show the validity of the following theorem which was applied in Appendix A.

Theorem. Under the conditions and in the notation of Lemma 2 there exists an orthonormal basis $\mathscr{B}$ of $\mathscr{S}$ of the form:

$$\mathscr{B} \equiv \{(u_1\ v_1)', (u_2\ v_2)', \ldots, (u_n\ v_n)', (v_1^*\ u_1^*)', (v_2^*\ u_2^*)', \ldots, (v_n^*\ u_n^*)'\}, \tag{B.6}$$

i.e. for any vector $(u\ v)'$ of the basis $\mathscr{B}$, the vector $(v^*\ u^*)'$ is one of the remaining $2n-1$ vectors in $\mathscr{B}$. In the case that the matrix $\mathscr{D}$ is real, the column m-vectors u_i and v_i $(i = 1, 2, \ldots, n)$ can be chosen to be real.

Proof. According to Lemma 2 there exists an orthonormal basis $\mathscr{B}'$ of $\mathscr{S}$ of the form (B.5), where the m-vectors t_i $(i = 1, 2, \ldots, 2n)$ can be chosen to be real in case the matrix $\mathscr{D}$ is real. Now for each $i = 1, 2, \ldots, n$ the pair of vectors $\{(t_i\ t_i^*)', (t_{n+i}\ -t_{n+1}^*)'\}$ of this basis $\mathscr{B}'$ yields an (orthonormal) pair in the orthonormal basis $\mathscr{B}$ to be found according to:

$$\begin{aligned}(u_i\ v_i)' &\equiv 2^{-1/2}(t_i + t_{n+i} \quad t_i^* - t_{n+i}^*)' \\ (v_i^*\ u_i^*)' &\equiv 2^{-1/2}(t_i - t_{n+i} \quad t_i^* + t_{n+i}^*)'.\end{aligned} \tag{B.7}$$

With this construction of the basis $\mathscr{B}$ we have proved the theorem.

Remark. The proof just given of the existence of an orthonormal basis $\mathscr{B}$ of $\mathscr{S}$ of the form (B.6) ($\mathscr{B}$ containing real vectors in the case that the matrix $\mathscr{D}$ is real), together with the proofs of Lemmas 1 and 2, suggests an algorithm which can be used in practice (e.g. in computer programs) for the actual calculation of such a basis.

Appendix C.

In this appendix we treat the problem raised in the last footnote in § 2. Using results and arguments out of Appendix B, we substantiate our assertion that in general no unique natural choice exists for the first and $(m+2)$-th column of $\tilde{\mathscr{T}}^\dagger$ in equation (2.12). The question seems interesting for a possible physical interpretation in actual physical problems of the construction operators $\tilde{\gamma}_r, \tilde{\gamma}_r^\dagger$ in equation (2.13) $(r = 1, 2, \ldots, m)$, associated with the remaining columns in $\tilde{\mathscr{T}}^\dagger$. We start with a lemma which helps to obtain a correct picture of the problem under consideration.

Lemma. Let

$$\mathscr{P}'' = \{\ell_1'', \ell_2''\} \equiv \{(t_1\ \eta_1 t_1^*)', (t_2\ \eta_2 t_2^*)'\} \tag{C.1}$$

be an orthonormal pair of $2m$-vectors and let $\mathscr{S}_{\text{pair}}$ be the 2-dimensional subspace

spanned by these vectors (η_1 and η_2 each denote 1 or -1). Then (1st statement) there is an infinite number of different pairs $\mathscr{P}$ of orthonormal vectors in $\mathscr{S}_{\text{pair}}$ of the form $\mathscr{P} \equiv \{\ell_1, \ell_2\} \equiv \{(u\ v)', (v^*\ u^*)'\}$. There is (2nd statement) at most one *real* orthonormal pair of that form in $\mathscr{S}_{\text{pair}}$ (it is self-evident that in this connection pairs are considered equal if each vector of one pair is proportional to a vector of the other pair). Finally (3rd statement) such a real pair exists if and only if there exists in $\mathscr{S}_{\text{pair}}$ a pair of vectors of the form (C.1), with ℓ_1'' and ℓ_2'' real and different η_1 and η_2.

Proof. The truth of the first statement is seen by observing that for each set of real scalars a and b with $a^2 + b^2 = 1$, one can construct a pair $\mathscr{P}$ of the required form lying in $\mathscr{S}_{\text{pair}}$ in the following way. Since the sign of η can always be changed by multiplication of the corresponding vector by the scalar i, we do not restrict the generality if we assume $\eta_1 = \eta_2 = 1$. Then also the orthonormal pair $\mathscr{P}_{ab}'' \equiv \{a\ell_1'' + b\ell_2'', b\ell_1'' - a\ell_2''\}$ has the form of the extreme right-hand side of equation (C.1) with $\eta_1 = \eta_2 = 1$ and consequently also $\mathscr{P}' \equiv \{\ell'_{ab1}, \ell'_{ab2}\} \equiv \{a\ell_1'' + b\ell_2'', \mathrm{i}(b\ell_1'' - a\ell_2'')\}$ has the same form but with $\eta_1 = 1$, $\eta_2 = -1$. The pair $\mathscr{P}_{ab} \equiv \{\ell_{ab1}, \ell_{ab2}\} \equiv \{2^{-1/2}(\ell'_{ab1} + \ell'_{ab2}), 2^{-1/2}(\ell'_{ab1} - \ell'_{ab2})\}$ is orthonormal, has the form $\{(u\ v)', (v^*\ u^*)'\}$ required for $\mathscr{P}$, and is obviously in general different for different combinations of a and b. The first statement has been proved.

Concentrating on the second statement, we suppose that $\mathscr{P}_1 \equiv \{(u_1\ v_1)', (v_1\ u_1)'\}$ and $\mathscr{P}_2 \equiv \{(u_2\ v_2)', (v_2\ u_2)'\}$ are two *real* orthonormal pairs of $2m$-vectors in $\mathscr{S}_{\text{pair}}$. We show that the pairs should be equal. Since the vectors $(u_1\ v_1)'$ and $(v_1\ u_1)'$ are perpendicular, the product $u_1^\dagger v_1 = v_1^\dagger u_1 = 0$. Since $(u_2\ v_2)'$ is a real vector in $\mathscr{S}_{\text{pair}}$, it is a linear combination of the two vectors in $\mathscr{P}_1$: $(u_2\ v_2)' = a(u_1\ v_1)' + b(v_1\ u_1)'$, with a and b real scalars. In view of the orthogonality of the vectors $(u_2\ v_2)'$ and $(v_2\ u_2)'$, the product $(au_1 + bv_1)^\dagger(av_1 + bu_1) = ab(u_1^\dagger u_1 + v_1^\dagger v_1) = ab$ should vanish. It follows that a or b equals zero. It is now easily shown that the pairs $\mathscr{P}_1$ and $\mathscr{P}_2$ are equal, indeed.

To prove the third statement we start from a real orthonormal pair $\mathscr{P}'' \equiv \{\ell_1'', \ell_2''\} \equiv \{(t_1\ t_1)', (t_2\ -t_2)'\}$ of vectors in $\mathscr{S}_{\text{pair}}$. We see immediately that the pair $\mathscr{P} \equiv \{2^{-1/2}(\ell_1'' + \ell_2''), 2^{-1/2}(\ell_1'' - \ell_2'')\} \equiv \{(u\ v)', (v\ u)'\}$ is a real orthonormal pair of vectors in $\mathscr{S}_{\text{pair}}$ of the form required for $\mathscr{P}$. The converse is also readily seen. With this also the last statement of the lemma has been proved.

We now turn our attention to the problem mentioned in the beginning of this appendix. In what follows we refer to the 1st and $(m+2)$-th column of $\tilde{\mathscr{T}}^\dagger$ in equation (2.12), which are assumed to be zero-eigenvalue eigenvectors of $\tilde{\mathscr{D}}^\dagger$ (cf the main text corresponding to the last footnote in § 2), as the ghost columns (of $\tilde{\mathscr{T}}^\dagger$); the vector $(100\ldots0\ 100\ldots0)'$, which is a zero-eigenvalue eigenvector of any $\tilde{\mathscr{D}}$ (cf the last footnote but one in § 2), is called the ghost vector. The ghost plane $\tilde{\mathscr{S}}_{\text{ghost}}$ is the 2-dimensional vector space spanned by the ghost columns of $\tilde{\mathscr{T}}^\dagger$.

In view of the lemma treated above, at most the ghost *plane* can be expected to be uniquely defined: the ghost *columns* themselves can be chosen in many ways in $\tilde{\mathscr{S}}_{\text{ghost}}$ unless it is considered reasonable to require the ghost columns to be real where possible. If λ_0 is the only λ_r vanishing in equation (2.13), $\tilde{\mathscr{S}}_{\text{ghost}}$ is obviously uniquely defined. However, in the case where other λ_r apart from λ_0 also vanish it is impossible to define a 2-dimensional space uniquely which can be considered as the natural one to contain the two ghost columns of $\tilde{\mathscr{T}}^\dagger$. This will now be shown.

It is natural to require for such a natural $\tilde{\mathscr{S}}_{\text{ghost}}$ that it contain the ghost vector $(100\ldots0\ 100\ldots0)'$. First we remark that there is no second such standard zero-eigenvalue eigenvector of $\tilde{\mathscr{D}}$ which can be given for a general $\tilde{\mathscr{D}}$ and which is derived by inspection from the special form (2.9) of $\tilde{\mathscr{D}}$. We show this by giving an example of a $\tilde{\mathscr{D}}$

where it is obvious that no such second vector exists. Let $\tilde{\mathscr{D}}$ be a grand-dynamical matrix of order 6 ($m = 2$) with the matrices $\tilde{A}$ and $\tilde{B}$ (defined in equation (2.9)) given by:

$$\tilde{A} \equiv \begin{pmatrix} 0 & M & M \\ M & A & 0 \\ M & 0 & C \end{pmatrix},$$

$$\tilde{B} \equiv \begin{pmatrix} 0 & M & M \\ -M & 0 & B \\ -M & -B & 0 \end{pmatrix}, \qquad A, B, C, M \text{ real numbers.} \tag{C.2}$$

It is seen by inspection that for general (real) values of the elements A, B, C and M a zero-eigenvalue eigenvector of $\tilde{\mathscr{D}}$ is given by:

$$[AC+B^2 \quad -2M(B+C) \quad 2M(B-A)$$
$$-(AC+B^2) \quad 2M(B+C) \quad -2M(B-A)]'. \tag{C.3}$$

Moreover equation (C.3) represents, in case $AC + B^2 \neq 0$, the only real zero-eigenvalue eigenvector of $\tilde{\mathscr{D}}$ of the form $(\tilde{t} \; -\tilde{t})'$ so that the multiplicity of the zero eigenvalue of $\tilde{\mathscr{D}}$ equals 2 (according to the proof of Lemma 2 in Appendix B, a higher multiplicity would imply the existence of at least two perpendicular real zero-eigenvalue eigenvectors of $\tilde{\mathscr{D}}$ of the form $(\tilde{t} \; -\tilde{t})'$ (cf equation (B.5))).

We now take $M \neq 0$ fixed and the elements A, B and $-C$ in the neighbourhood of the fixed value 1. For such a $\tilde{\mathscr{D}}$ we look for a second zero-eigenvalue eigenvector which is as standard as the ghost vector and perpendicular to this vector. If $AC + B^2 \neq 0$, such a second vector is given uniquely by equation (C.3) (apart from a multiplicative scalar). However, we obtain a different result in case $AC + B^2 = 0$. As an example we consider $\tilde{\mathscr{D}}^0$, by which we denote the $\tilde{\mathscr{D}}$ under consideration with the fixed M chosen and $A = B = -C = 1$. The existence of a second standard zero-eigenvalue eigenvector for this $\tilde{\mathscr{D}}^0$ would imply at least that the limiting vector of the normalised vector proportional to equation (C.3) for the elements A, B and $-C$ tending to 1 (M fixed), together with the ghost vector, uniquely defines a ghost plane connected with $\tilde{\mathscr{D}}^0$. However, the ghost plane thus obtained is not unique, which is seen e.g. by considering the cases $A = B = 1$, $C \to -1$ (limiting vector $\propto (1 \; -2M \; 0 \qquad -1 \; 2M \; 0)'$) and $B = -C = 1$, $A \to 1$ (limiting vector $\propto (1 \; 0 \; 2M \qquad -1 \; 0 \; -2M)'$). (Note that the ghost vector and the two limiting vectors just mentioned constitute a set of three linearly independent zero-eigenvalue eigenvectors of $\tilde{\mathscr{D}}^0$, which easily leads us to the conclusion that the multiplicity of the zero eigenvalue equals 4.) Therefore at least for $\tilde{\mathscr{D}}^0$ no second standard zero-eigenvalue eigenvector exists, which we wanted to show initially. Simultaneously we have seen that a natural ghost plane does not exist either for $\tilde{\mathscr{D}}^0$. Apparently the existence of a second standard zero-eigenvalue eigenvector or of a natural ghost plane of such eigenvectors is not a general property of any $\tilde{\mathscr{D}}$ on the basis of its special form (2.9) alone.

In view of this result it is impossible (in case λ_r other than λ_0 are also vanishing) to define uniquely the plane $\tilde{\mathscr{S}}_{\text{ghost}}$ that can be considered as the natural one to contain the two ghost columns of $\tilde{\mathscr{T}}^\dagger$. The only 'natural' requirement on the plane $\tilde{\mathscr{S}}_{\text{ghost}}$ in this case is that the ghost vector lies in it. Accordingly for the construction of the ghost columns of $\tilde{\mathscr{T}}^\dagger$ we can start from any orthonormal pair of the form $\tilde{\mathscr{P}}'' \equiv \{2^{-1/2}(100\ldots0 \; 100\ldots0)', (\tilde{t}_2 \; \eta_2 \tilde{t}_2^*)'\}$; each $\tilde{\mathscr{B}}'$ (equation (B.5)) for example, with the (normalised) ghost vector as one of the vectors, immediately yields $2n - 1$ such pairs.

According to the procedure outlined in the proof of the first statement of the lemma above, we can in many ways construct from the $\tilde{\mathcal{P}}''$ chosen a pair of ghost columns of $\tilde{\mathcal{T}}^{\dagger}$ of the form $\{(\tilde{u}\ \tilde{v})', (\tilde{v}^*\ \tilde{u}^*)'\}$.

To summarise, we conclude that in actual physical problems the physical interpretation of the construction operators $\tilde{\gamma}_r$, $\tilde{\gamma}_r^{\dagger}$ in equation (2.13) ($r = 1, 2, \ldots, m$) at least in cases of a vanishing λ_r (again $r \neq 0$) should be derived by physical arguments and that the mathematics of the problem alone does not give answers. For example, let a physical Hamiltonian have temperature-dependent coefficients, and let this Hamiltonian at a certain critical temperature T_c have some $\lambda_r = 0$. It may then happen that for the Hamiltonian at T_c only transformation matrices $\tilde{\mathcal{T}}^{\dagger}(T_c)$, which are obtained as the limit of $\tilde{\mathcal{T}}^{\dagger}(T)$ for the temperature T tending to T_c, have columns which correspond by equation (2.11) to physically meaningful $\tilde{\gamma}$.

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