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LETTER TO THE EDITOR

Generalized Bogolyubov transformation

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Abstract. The Bogolyubov transformation, frequently used in dealing with pairing interactions of fermions, is extended to allow for binary coupling between any (even) number of fermions by using a matrix transformation 'coefficient'. The corresponding quasiparticles and quasi-vacuum state are derived. The normally ordered expansion of the unitary generalized Bogolyubov operator is obtained by application of the technique of integration within an ordered product (IWOP) for the fermion system.

Bogolyubov transformations [1, 2] are very useful in dealing with the pairing interactions of fermions in superconductivity theory, nuclear physics and quantum chemistry. The unitary operator that generates the Bogolyubov transformation used in coupling two fermions is

$$V(\lambda)=\exp(\lambda a_1 a_2-\lambda^* a_2^\dagger a_1^\dagger). \tag{1}$$

In this work we investigate the transformation for multiple fermions. We shall derive the normally ordered form of the following unitary operator

$$U(\Lambda)=\exp[\tfrac{1}{2}(a_i\Lambda_{ij}a_j-a_i^\dagger\Lambda_{ij}^\dagger a_j^\dagger)] \tag{2}$$

which, as will be shown, generates the Bogolyubov transformation whose 'coefficient' is a matrix. In (2), a_i ($a_j^\dagger$) are fermion annihilation (creation) operators whose indices run from 1 to n and summation over repeated indices is assumed. The matrix Λ_{ij} must of course be antisymmetric which requires the number n to be even in order that Λ have an inverse. We restrict our considerations to matrices Λ having this form.

In this letter we investigate how the fermion operators transform under U. The quasiparticle vacuum state is derived. Finally, with the aid of the technique of integration within an ordered product (IWOP) [3–5] and making use of the fermion coherent state [6] we derive the normal product form of U.

We begin our investigation of the mapping (2) by calculating its effect on the annihilator of the multimode fermion vacuum state.

Using the anticommutator result

$$\{a_i, a_j^\dagger\}=\delta_{ij} \tag{3}$$

and the identities

$$\begin{aligned} &\mathrm{e}^{A}B\,\mathrm{e}^{-A}=B+[A,B]+\frac{1}{2!}[A,[A,B]]+\frac{1}{3!}[A,[A,[A,B]]]+\dots\\ &[A,B,C]=A\{B,C\}-\{A,C\}B \end{aligned} \tag{4}$$

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we obtain

$$Ua_i^\dagger U^{-1} = a_j^\dagger[\cos(\Lambda^\dagger\Lambda)^{1/2}]_{ji} + a_j[\Lambda(\Lambda^\dagger\Lambda)^{-1/2}\sin(\Lambda^\dagger\Lambda)^{1/2}]_{ji} \tag{5}$$

$$= a_j^\dagger[\cos(\Lambda^\dagger\Lambda)^{1/2}]_{ji} + a_j[\sin(\Lambda\Lambda^\dagger)^{1/2}(\Lambda\Lambda^\dagger)^{-1/2}\Lambda]_{ji}. \tag{6}$$

As shown in [6], an arbitrary non-singular matrix can always be decomposed as the product of a Hermitian matrix H and a unitary matrix, which we take as e^{iF}. Then in a fashion analogous to the polar representation of complex numbers, we may in general write

$$\Lambda = H\,e^{iF} \tag{7}$$

with $H^\dagger = H$ and $F^\dagger = F$, giving

$$\Lambda\Lambda^\dagger = H^2. \tag{8}$$

From the required antisymmetry of Λ we have $\Lambda = -\tilde{\Lambda}$ which gives

$$\Lambda = -e^{i\tilde{F}}\tilde{H} \qquad \Lambda^\dagger\Lambda = \tilde{H}^2 = e^{-iF}H^2\,e^{iF} \qquad \tilde{H}^2\,e^{-iF} = e^{-iF}H^2. \tag{9}$$

These relations suffice to find H and e^{iF}.

Substituting (8) and (9) into expressions (5) and (6) we simplify the latter to obtain the quasiparticle creation ($a_i^{\dagger\prime}$) and annihilation ($a_i^\prime$) operators

$$a_i^{\dagger\prime} = Ua_i^\dagger U^{-1} = a_j^\dagger(\cos\tilde{H})_{ji} - a_j(e^{i\tilde{F}}\sin\tilde{H})_{ji} \tag{10}$$

$$= a_j^\dagger(\cos\tilde{H})_{ji} + a_j(\sin H\,e^{iF})_{ji}. \tag{11}$$

It follows that

$$a_i^\prime = Ua_iU^{-1} = a_j(\cos H)_{ji} + a_j^\dagger(\sin\tilde{H}\,e^{-i\tilde{F}})_{ji} \tag{12}$$

$$= a_j(\cos H)_{ji} - a_j^\dagger(e^{-iF}\sin H)_{ji}. \tag{13}$$

We have used the antisymmetry of $e^{-iF}\sin H$ to go from (12) to (13).

We now seek the quasiparticle vacuum state $U|\vec{0}\rangle \equiv \|\vec{0}\rangle$ annihilated by $a_l^\prime$, where $|\vec{0}\rangle$ is the multifermion vacuum state annihilated by a_l

$$a_l|\vec{0}\rangle = 0 \qquad l = 1, 2, \ldots, n. \tag{14}$$

We first obtain an equation satisfied by $\|\vec{0}\rangle$ by allowing a_l to operate on $\|\vec{0}\rangle$,

$$a_l\|\vec{0}\rangle = UU^{-1}a_lU|\vec{0}\rangle \tag{15}$$

which we then solve to obtain $\|\vec{0}\rangle$.

As a consequence of (11) and (13) we can, noting that $U^{-1}(\Lambda) = U(-\Lambda)$, rewrite (15) as

$$\begin{aligned} a_l\|\vec{0}\rangle &= U[a_j(\cos H)_{jl} + a_j^\dagger(e^{-iF}\sin H)_{jl}]|\vec{0}\rangle \\ &= Ua_j^\dagger(e^{-iF}\sin H)_{jl}U^{-1}U|\vec{0}\rangle \\ &= [a_j^\dagger(\cos\tilde{H}\,e^{-iF}\sin H)_{jl} + a_j(\sin^2 H)_{jl}]\|\vec{0}\rangle \end{aligned} \tag{16}$$

and simplified with the aid of (9) to give

$$a_l\|\vec{0}\rangle = a_j^\dagger(e^{-iF}\tan H)_{jl}\|\vec{0}\rangle. \tag{17}$$

This is the required equation for $\|\vec{0}\rangle$ which may be solved by noting that

$$a_j^\dagger(e^{-iF}\tan H)_{jl}\exp(-\tfrac{1}{2}a_i^\dagger(e^{-iF}\tan H)_{ij}a_j^\dagger) = \{a_l, \exp[-\tfrac{1}{2}a_i(e^{-iF}\tan H)_{ij}a_j^\dagger]\}.$$

The solution for $\|\vec{0}\rangle$ is then:

$$\|\vec{0}\rangle = C\exp[-\tfrac{1}{2}a_i^\dagger(e^{-iF}\tan H)_{ij}a_j^\dagger]|\vec{0}\rangle. \tag{18}$$

The normalization coefficient C can be obtained by calculating the norm

$$1=\langle\tilde{0}\|\tilde{0}\rangle=|C|^2\langle\tilde{0}|\exp[-\tfrac{1}{2}a_i(\tan H\,\mathrm{e}^{\mathrm{i}F})_{ij}a_j]\exp[-\tfrac{1}{2}a_i^\dagger(\mathrm{e}^{-\mathrm{i}F}\tan H)_{ij}a_j^\dagger]|\tilde{0}\rangle. \qquad (19)$$

For this purpose we introduce the fermion coherent state [7] $|\vec{\alpha}\rangle\equiv\Pi_i|\alpha\rangle$ (repeated indices do not imply summation in (20)-(23)) with

$$|\alpha_i\rangle=\exp[-\tfrac{1}{2}\bar{\alpha}_i\alpha_i+a_i^\dagger\alpha_i]|0\rangle_i \qquad a_i|\alpha_i\rangle=\alpha_i|\alpha_i\rangle \qquad (20)$$

$$\langle\alpha_i|={}_i\langle 0|\exp[-\tfrac{1}{2}\bar{\alpha}_i\alpha_i+\bar{\alpha}_i a_i] \qquad \langle\alpha_i|a_i^\dagger=\langle\alpha_i|\bar{\alpha}_i \qquad (21)$$

where α_i is a Grassmann number [8] with the properties

$$\alpha_i\bar{\alpha}_i+\alpha_i\bar{\alpha}_i=0 \qquad \alpha_i^2=0 \qquad \bar{\alpha}_i^2=0 \qquad (22)$$

$$\int \mathrm{d}\alpha_i=0 \qquad \int \mathrm{d}\alpha_i\,\alpha_i=1 \qquad \int \mathrm{d}\bar{\alpha}_i=0 \qquad \int \mathrm{d}\bar{\alpha}_i\,\bar{\alpha}_i=0. \qquad (23)$$

Consistency requires that the α_i anticommute with a_i and $a_i^\dagger$ also.

Let η_i and $\bar{\eta}_i$ also be Grassmann numbers then the following formulae may be obtained for A a complex-valued $n\times n$ matrix:

$$\int\prod_i \mathrm{d}\bar{\alpha}_i\,\mathrm{d}\alpha_i\,\exp\{-\bar{\alpha}_iA_{ij}\alpha_j+\bar{\alpha}_i\eta_i+\bar{\eta}_i\alpha_i\}=(\det A)\exp\{\bar{\eta}_i(A^{-1})_{ij}\eta_j\} \qquad (24)$$

while for $B=\begin{pmatrix}A_{11}&A_{12}\\A_{21}&A_{22}\end{pmatrix}$, a $2n\times 2n$ matrix whose elements A_{11}, A_{12}, A_{21} and A_{22} are $n\times n$ submatrices,

$$\int\prod_i \mathrm{d}\bar{\alpha}_i\,\mathrm{d}\alpha_i\,\exp\left\{\tfrac{1}{2}(\alpha,\bar{\alpha})\begin{pmatrix}A_{11}&A_{12}\\A_{21}&A_{22}\end{pmatrix}\begin{pmatrix}\alpha\\\bar{\alpha}\end{pmatrix}+(\bar{\eta},\eta)\begin{pmatrix}\alpha\\\bar{\alpha}\end{pmatrix}\right\}$$
$$=\left[\det\begin{pmatrix}A_{11}&A_{12}\\A_{21}&A_{22}\end{pmatrix}\right]^{1/2}\exp\left[\tfrac{1}{2}(\bar{\eta},\eta)\begin{pmatrix}A_{21}&A_{22}\\A_{11}&A_{12}\end{pmatrix}^{-1}\begin{pmatrix}\eta\\\bar{\eta}\end{pmatrix}\right] \qquad (25)$$

where $(\alpha,\bar{\alpha})=(\alpha_1,\alpha_2,\ldots,\alpha_n;\bar{\alpha}_1,\bar{\alpha}_2,\ldots,\bar{\alpha}_n)$.

Using (25) and the IWOP technique and the completeness relation of the fermion coherent state, $|\alpha_i\rangle$ can be put into normal product form [9]

$$\int\prod_i \mathrm{d}\bar{\alpha}_i\,\mathrm{d}\alpha_i|\vec{\alpha}\rangle\langle\vec{\alpha}|=\int\prod_i \mathrm{d}\bar{\alpha}_i\,\mathrm{d}\alpha_i:\exp(-\bar{\alpha}_i\alpha_i+a_i^\dagger\alpha_i+\bar{\alpha}_ia_i-a_i^\dagger a_i):=1 \qquad (26)$$

where : : denotes the normal product and we have used

$$|\vec{0}\rangle\langle\vec{0}|=:\mathrm{e}^{-a_i^\dagger a_i}:. \qquad (27)$$

Using (20), (21), (25) and (26) we can evaluate (19) to obtain

$$1=|C|^2\langle 0|\int\prod_i \mathrm{d}\bar{\alpha}_i\,\mathrm{d}\alpha_i$$
$$\times:\exp\left\{\tfrac{1}{2}(\alpha,\bar{\alpha})\begin{pmatrix}-\tan H\,\mathrm{e}^{\mathrm{i}F}&\mathbb{1}\\-\mathbb{1}&-\mathrm{e}^{-\mathrm{i}F}\tan H\end{pmatrix}\begin{pmatrix}\alpha\\\bar{\alpha}\end{pmatrix}\right.$$
$$\left.+(a^\dagger-a)\begin{pmatrix}\alpha\\\bar{\alpha}\end{pmatrix}-a_i^\dagger a_i\right\}:|0\rangle$$
$$=|C|^2\sqrt{\det(\sec^2 H)}.$$

Therefore, up to an arbitrary phase factor

$$C=\sqrt{\det(\cos H)}. \qquad (28)$$

Although $a_i^2 = a_i^{\dagger 2} = 0$, the normal product form of U for $n \neq 2$ is not immediately obvious. In the following, we exploit the fermion coherent state and the IWOP technique to derive the normal product expression for U.

Let U operate on $|\vec{\alpha}\rangle$ giving

$$U|\vec{\alpha}\rangle = U \exp(a_i^\dagger \alpha_i) U^{-1} U|\vec{0}\rangle \exp(-\tfrac{1}{2}\bar{\alpha}_i\alpha_i)$$
$$= \exp\{a_j^\dagger(\cos \tilde{H})_{ji}\alpha_i + a_j(\sin H\, \mathrm{e}^{\mathrm{i}F})_{ji}\alpha_i\} \sqrt{\det(\cos H)}$$
$$\times \exp[-\tfrac{1}{2}a_i^\dagger(\mathrm{e}^{-\mathrm{i}F} \tan H)_{ij}a_j^\dagger]|\vec{0}\rangle \exp(-\tfrac{1}{2}\bar{\alpha}_i\alpha_i). \tag{29}$$

Using the Baker-Hausdorff formula and (4) we can decompose the first exponential in (29)

$$\exp\{\ldots\} = \exp[-\alpha_i(\cos H)_{ij}a_j^\dagger] \exp[a_j(\sin H\, \mathrm{e}^{\mathrm{i}F})_{ji}\alpha_i] \exp[\tfrac{1}{4}\alpha_i(\sin 2H\, \mathrm{e}^{\mathrm{i}F})_{ij}\alpha_j]. \tag{30}$$

Therefore (29) becomes

$$U|\vec{\alpha}\rangle = \sqrt{\det(\cos H)} \exp[-\tfrac{1}{2}\bar{\alpha}_i\alpha_i - \alpha_i(\sec H)_{ij}a_j^\dagger$$
$$+ \tfrac{1}{2}\alpha_i(\tan H\, \mathrm{e}^{\mathrm{i}F})_{ij}\alpha_j - \tfrac{1}{2}a_i^\dagger(\mathrm{e}^{\mathrm{i}F} \tan H)_{ij}a_j^\dagger]|\vec{0}\rangle. \tag{31}$$

By virtue of (26) and the IWOP technique we can put U into the form

$$U = \int \prod_i \mathrm{d}\bar{\alpha}_i\, \mathrm{d}\alpha_i\, U|\vec{\alpha}\rangle\langle\vec{\alpha}|$$
$$= \sqrt{\det(\cos H)} \int \mathrm{d}\bar{\alpha}_i\, \mathrm{d}\alpha_i :\exp\{-\bar{\alpha}_i\alpha_i - \alpha_i(\sec H)_{ij}a_j^\dagger + \bar{\alpha}_i a_i$$
$$+ \tfrac{1}{2}\alpha_i(\tan H\, \mathrm{e}^{F})_{ij}\alpha_j - \tfrac{1}{2}a_i^\dagger(\mathrm{e}^{-F} \tan H)_{ij}a_j^\dagger - a_i^\dagger a_i\}: \tag{32}$$
$$= \sqrt{\det(\cos H)} \int \prod_i \mathrm{d}\bar{\alpha}_i\, \mathrm{d}\alpha_i :\exp\left\{\tfrac{1}{2}(\alpha, \bar{\alpha})\begin{pmatrix}\tan H\, \mathrm{e}^{\mathrm{i}F} & \mathbb{I} \\ -\mathbb{I} & 0\end{pmatrix}\begin{pmatrix}\alpha \\ \bar{\alpha}\end{pmatrix}\right.$$
$$\left. + (a^\dagger \sec \tilde{H}, -a)\begin{pmatrix}\alpha \\ \bar{\alpha}\end{pmatrix} - a_i^\dagger a_i - \tfrac{1}{2}a_i^\dagger(\mathrm{e}^{-\mathrm{i}F} \tan H)_{ij}a_j^\dagger\right\}:. \tag{33}$$

Using

$$\begin{pmatrix}A & B \\ C & D\end{pmatrix}^{-1} = \begin{pmatrix}(A - BD^{-1}C)^{-1} & A^{-1}B(CA^{-1}B - D)^{-1} \\ D^{-1}C(BD^{-1}C - A)^{-1} & (D - CA^{-1}B)^{-1}\end{pmatrix}$$

we finally write (33) as

$$U = \sqrt{\det(\cos H)} \exp\{-\tfrac{1}{2}a_i^\dagger(\mathrm{e}^{-\mathrm{i}F} \tan H)_{ij}a_j^\dagger\} :\exp\{a_i^\dagger(\sec \tilde{H} - \mathbb{I})_{ij}a_j\}:$$
$$\times \exp\{\tfrac{1}{2}a_i(\tan H\, \mathrm{e}^{\mathrm{i}F})_{ij}a_j\} \tag{34}$$

which is the normal product form of U.

In summary, we have extended the formalism of Bogolyubov transformations to that where the parameter is an antisymmetric matrix. The corresponding vacuum state and quasiparticles as well as the normal form of the transformation are derived by the IWOP technique. This formalism is likely to prove useful in tackling many-fermion systems, as we hope to show in the near future.

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