On the Mathematical Structure of the New-Tamm-Dancoff Procedure

I. Mathematical Basis

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The New Tamm-Dancoff method is a procedure for the approximate determination of differences of eigenvalues in quantum field theory. This procedure can be formulated mathematically in the framework of the theory of C*-algebras, especially in our case by using von Neumann's infinite tensor products. Calculational rules are presented for operators which obey the canonical anticommutation relations. The concept of the CAR tensor product is introduced for the joint treatment of a system algebra and the associated functional algebra. A conjugation is discussed which will be needed for a proof of equivalence in II.

I. Mathematical Basis

The present paper prepares the discussion of the New-Tamm-Dancoff-procedure (NTD-procedure) in non-relativistic many-particle physics *. This NTD-procedure permits the treatment of collective phenomena by transformations with respect to macroscopically different ground states. These transformations can be formulated within the mathematical context of C*-algebras, especially in our case by the use of von Neumann infinite tensor products. As these mathematical tools are quite evident, but not generally in use, we collect the main results of the theory in § 1 taking into account the physical interpretations.

We will use extensively computational rules for operators which obey the canonical anticommutation relations (CAR). In § 2 we present a calculus simplifying these computations.

In addition to the usual creation- and annihilation operators of the physical system under consideration, the NTD-procedure makes use of creation- and annihilation operators of the so-called functional algebra. In § 3 we explain how the system and the functional algebra can be treated together by using the CAR-tensor product.

In the analysis of the NTD-procedure a conjugation in Fock space will appear. The main properties of such conjugations are treated in § 4; it will be shown that the physical interpretation is the same using the original or the conjugate system.

§ 1. Infinite Tensor Products and the CAR-algebra

Let the position- and spin coordinates constitute the configuration space Γ; e.g. $\Gamma = \mathbb{R}^3 \times \{-\frac{1}{2}, \frac{1}{2}\}$ for the case of spin 1/2 fermions. We also consider bounded open subsets V of Γ, the so-called local regions. One-particle quantum mechanics is formulated by use of the Hilbert space $L^2(\Gamma)$ for the global system and $L^2(V)$ for the local systems respectively. For later discussions it is advantageous also to consider finite-dimensional one-particle Hilbert spaces. For this purpose we start with the spectral decomposition $E(\varepsilon)$ (with energy ε) of the one-particle Hamiltonian of the local region V. Given a fixed cut-off energy ε_0, $E(\varepsilon_0) L^2(V)$ is the Hilbert space including all state vectors for which any single measurement of energy has a result $\leqq \varepsilon_0$. This space is finite-dimensional for the physical models relevant to our considerations.

In all three cases the one-particle Hilbert space $\mathscr{C}$ ($L^2(\Gamma)$, $L^2(V)$ or $E(\varepsilon_0) L^2(V)$) is separable. Thus we can find a complete orthonormal system $(w_\nu)_{\nu \in \mathscr{N}}$ in $\mathscr{C}$. Here $\mathscr{N}$ is the set of the positive integers $\mathbb{N}$ or some set $\{1, 2, \ldots, n\}$.

According to the Pauli principle, each one-particle state of an orthonormal system can at most be occupied by one fermion. So we introduce for each w_ν

* See: On the Mathematical Structure of the New-Tamm-Dancoff-Procedure: II. Functional Quantum Mechanics and the Equivalence with a Product of Schrödinger Problems [9].

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the states $\begin{pmatrix}0\\1\end{pmatrix}_\nu$ and $\begin{pmatrix}1\\0\end{pmatrix}_\nu$ which denote an occupied or unoccupied one-particle state w_ν respectively. They span a two-dimensional Hilbert space $\mathbb{C}_\nu^2$. We consider the spaces $\mathbb{C}_\nu^2$, $\nu \in \mathcal{N}$ as Hilbert spaces for the description of independent quantum mechanical systems with two degrees of freedom. The collective description of all these systems is given by a many-particle state vector

$$\Psi = \bigotimes_{\nu \in \mathcal{N}} \begin{pmatrix}\alpha_\nu\\ \beta_\nu\end{pmatrix} \quad \text{with} \quad |\alpha_\nu|^2 + |\beta_\nu|^2 = 1. \tag{1.1}$$

The transition probability between two such states is the square of the transition amplitude

$$\langle \Psi' | \Psi'' \rangle = \prod_{\nu \in \mathcal{N}} (\bar{\alpha}_\nu' \alpha_\nu'' + \bar{\beta}_\nu' \beta_\nu''). \tag{1.2}$$

In the case $\mathcal{N} = \mathbb{N}$ the convergence of the infinite product is not given in general. We can understand this even from the physical point of view. Transition amplitudes $\neq 0$ can only be expected between two states, if they are essentially different for at most a finite number of their constituents $\begin{pmatrix}\alpha_\nu\\ \beta_\nu\end{pmatrix}$. We follow von Neumann [1] and choose a fixed reference vector

$$\Psi = \bigotimes_{\nu \in \mathcal{N}} \begin{pmatrix}\alpha_\nu\\ \beta_\nu\end{pmatrix}; \quad |\alpha_\nu|^2 + |\beta_\nu|^2 = 1.$$

For two state vectors

$$\Psi' = \bigotimes_{\nu \in \mathcal{N}} \begin{pmatrix}\alpha_\nu'\\ \beta_\nu'\end{pmatrix} \quad \text{and} \quad \Psi'' = \bigotimes_{\nu \in \mathcal{N}} \begin{pmatrix}\alpha_\nu''\\ \beta_\nu''\end{pmatrix}$$

with

$$\begin{pmatrix}\alpha_\nu'\\ \beta_\nu'\end{pmatrix} = \begin{pmatrix}\alpha_\nu\\ \beta_\nu\end{pmatrix} = \begin{pmatrix}\alpha_\nu''\\ \beta_\nu''\end{pmatrix}$$

for all but a finite number of $\nu \in \mathcal{N}$, the product (1.2) now becomes well defined. This product can be extended sesquilinearly to the linear hull of states of type Ψ' and Ψ'' and it is positive definite if state vectors with equal transition amplitudes (to any other state vector) are identified. The completion of the pre-Hilbert space obtained this way is — unfortunately, historically in contrast to the space mentioned in (1.5) — called the *incomplete direct product space* (IDPS) of the spaces $\mathbb{C}_\nu^2$ with respect to the reference vector Ψ and is denoted by

$$\mathcal{H}_\Psi = \bigotimes_{\nu \in \mathcal{N}}^{\Psi} \mathbb{C}_\nu^2. \tag{1.3}$$

An important special case is the Fock space. Here we start with the reference vector

$$\Omega = \bigotimes_{\nu \in \mathcal{N}} \begin{pmatrix}1\\0\end{pmatrix},$$

the so-called "bare vacuum". The corresponding IDPS $\mathcal{H}_\Omega$ is identical with the fermion Fock space of Cook [2].

As was shown by von Neumann [1], the spaces $\mathcal{H}_\Psi$ and $\mathcal{H}_{\Psi'}$ are identical iff the corresponding reference vectors Ψ and Ψ' are strongly equivalent, i.e. if they fulfill the condition

$$\sum_{\nu \in \mathcal{N}} |1 - \bar{\alpha}_\nu \alpha_\nu' - \bar{\beta}_\nu \beta_\nu'| < \infty. \tag{1.4}$$

The direct sum of all IDPS's with respect to the classes of strongly equivalent vectors is called the "complete direct product space":

$$\mathcal{H} := \bigoplus_{\substack{\text{all strong}\\ \text{equivalence classes}}} \mathcal{H}_{\Psi}. \tag{1.5}$$

Given a fixed IDPS $\mathcal{H}_\Psi$ we consider the operators

$$a_\nu = \begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix} \otimes \cdots \otimes \begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix} \otimes \underbrace{\begin{pmatrix}0 & 1\\ 0 & 0\end{pmatrix}}_{\nu\text{th factor}} \otimes \begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix} \otimes \cdots \tag{1.6}$$

and

$$a_\nu^+ = \begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix} \otimes \cdots \otimes \begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix} \otimes \underbrace{\begin{pmatrix}0 & 0\\ 1 & 0\end{pmatrix}}_{\nu\text{th factor}} \otimes \begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix} \otimes \cdots. \tag{1.7}$$

a_ν has the meaning of an annihilation, a_ν^+ that of a creation operator for the one-particle state w_ν. It is easy to verify the canonical anticommutator relations (CAR) for the operator families $(a_\nu)_{\nu \in \mathcal{N}}$ and $(a_\nu^+)_{\nu \in \mathcal{N}}$:

$$\begin{aligned} \{a_\mu, a_\nu^+\} &= \delta_{\mu\nu} I; \\ \{a_\mu, a_\nu\} &= \{a_\mu^+, a_\nu^+\} = 0. \end{aligned} \tag{1.8}$$

Thus they have the operator norms

$$\|a_\mu\| = \|a_\mu^+\| = 1 \quad [3].$$

They generate a subalgebra of the algebra of all bounded operators $\mathcal{L}(\mathcal{H}_\Psi)$. The completion of this subalgebra with respect to the operator norm is denoted by $\mathfrak{A}_\Psi$. If $\mathcal{H}_{\Psi'}$ is another IDPS and $\mathfrak{A}_{\Psi'}$

the associated algebra, then $\mathfrak{A}_\Psi$ and $\mathfrak{A}_{\Psi'}$ are canonically isomorphic [4]. Therefore, $\mathfrak{A}_\Psi$ and $\mathfrak{A}_{\Psi'}$ can be considered as different representations of a fixed C*-algebra $\mathfrak{A}$, called the algebra of the canonical anticommutation relations (*CAR-algebra*).

According to Klauder, McKenna and Woods [5], two IDPS representations of $\mathfrak{A}$ are unitarily equivalent (i.e. they describe the same physical situation), if the corresponding reference vectors satisfy the condition

$$\sum_{\nu\in\mathcal{N}} |1 - |\bar{\alpha}_\nu \alpha_\nu' + \bar{\beta}_\nu \beta_\nu'|| < \infty . \tag{1.9}$$

Such vectors are called weakly equivalent. In the case $\mathcal{N} = \mathbb{N}$ there are still non-countable many unitarily inequivalent representations of $\mathfrak{A}$ describing macroscopically different physical phenomena.

For a fixed representation the observables of a physical system are given by those selfadjoint operators, which can be approximated by elements of $\mathfrak{A}_\Psi$ in the sense of strong resolvent convergence [6, I]. They are called affiliated to the representation $\mathfrak{A}_\Psi$ of $\mathfrak{A}$ in $\mathscr{H}_\Psi$. In the cases under consideration these operators can be given by expansions of the form

$$H = \sum_{m\in\mathbb{N}} \sum_{n\in\mathbb{N}} \sum_{\mu_1,\ldots,\mu_m\in\mathcal{N}} \sum_{\nu_1,\ldots,\nu_n\in\mathcal{N}} h_{\mu_1\ldots\mu_m\nu_1\ldots\nu_n} \cdot a_{\mu_1}^+ \ldots a_{\mu_m}^+ a_{\nu_1} \ldots a_{\nu_n} . \tag{1.10}$$

Here convergence is considered pointwise with respect to states from a suitable domain (for special cases see [7]). The general treatment of operators of type (1.10) needs further mathematical prerequisites which are not in the scope of this paper.

E.g. let us consider the number-operator needed later

$$\mathscr{Z} := \sum_{\nu\in\mathcal{N}} a_\nu^+ a_\nu . \tag{1.11}$$

The series defining $\mathscr{Z}$ can be applicated to any vector

$$\Psi = \sum_{m\in\mathbb{N}} \sum_{\mu_1<\cdots<\mu_m} \psi_{\mu_1\ldots\mu_m} a_{\mu_1}^+ \ldots a_{\mu_m}^+ \Omega$$

in Fock space, which satisfies

$$\sum_{m\in\mathbb{N}} \sum_{\mu_1<\cdots<\mu_m} m^2 |\psi_{\mu_1\ldots\mu_m}|^2 < \infty .$$

§ 2. Computational Rules for CAR-operators

The following calculus is motivated by the frequent occurrence of operator products like $a_{\mu_1}^+ \ldots a_{\mu_m}^+$: Let $A := (A_\mu)_{\mu\in\mathcal{N}}$, $B = (B_\mu)_{\mu\in\mathcal{N}}$, ... be families of operators in $\mathfrak{A}$. The sum, scalar multiple, product, and adjoint of such families are defined in components, e.g. $\alpha A + \beta B := (\alpha A_\mu + \beta B_\mu)_{\mu\in\mathcal{N}}$. Further let $I = (I)_{\mu\in\mathcal{N}}$, $0 = (0)_{\mu\in\mathcal{N}}$.

For an operator family A and a finite subset $M \subseteqq \mathcal{N}$ let

$$A^M := A_{\mu_1} \ldots A_{\mu_m} , \tag{2.1}$$

with $\mu_1 < \mu_2 < \cdots < \mu_m$ being the indices of M in their natural order.

With the definitions above we have for instance

$$(\alpha A + B^+)^M = (\alpha A_{\mu_1} + B_{\mu_1}^+) \cdot (\alpha A_{\mu_2} + B_{\mu_2}^+) \ldots (\alpha A_{\mu_m} + B_{\mu_m}^+) .$$

Expanding a state Ψ of the Fock space with respect to the canonical orthonormal system associated with the creation operator family $a^+ = (a_\mu{}^+)_{\mu\in\mathcal{N}}$ gives the suggestive formula

$$\Psi = \sum_{\substack{M\subseteqq\mathcal{N}\\ M \text{ finite}}} a^{+M}\Omega \langle a^{+M}\Omega \,|\, \Psi\rangle . \tag{2.2}$$

The operator series (1.10) can be written

$$H = \sum_{\substack{M,N\subseteqq\mathcal{N}\\ M,N \text{ finite}}} h_{MN}\, a^{+M} a^N \tag{2.3}$$

with the notation $h_{MN} := h_{\mu_1\ldots\mu_m\nu_1\ldots\nu_n}$.

Calculations with CAR-operators frequently require the normal ordering of a product of the form $a^{+M} a^N a^{+P}$. The rules collected in the following are useful for this purpose.

We still need for a finite subset

$$M = \{\mu_1, \ldots, \mu_m\} \subseteqq \mathcal{N}$$

the power $|M| = m$ and, if $N = \{\nu_1, \ldots, \nu_n\} \subseteqq \mathcal{N}$ is another finite subset, the signum of the two sets

$$\operatorname{sign}(M|N) := \begin{cases} 0, & \text{if } M \cap N \neq \emptyset, \\ \text{signum of the permutation necessary to transform} \\ \mu_1, \ldots, \mu_m, \nu_1, \ldots, \nu_n, \text{ in the natural order } \varrho_1 < \cdots < \varrho_{m+n} \\ \text{if } M \cap N = \emptyset . \end{cases} \tag{2.4}$$

Simple combinatorial calculations are used to prove

Lemma 2.1. (*Calculation rules for the signum*)

For finite subsets M, N, $P \subseteqq \mathcal{N}$ *the following relations hold*:

$$\operatorname{sign}(M\,|\,N) = (-1)^{|M|\cdot|N|}\operatorname{sign}(N\,|\,M), \tag{2.5a}$$

$$\operatorname{sign}(M\,|\,P)\operatorname{sign}(M\cup P\,|\,N) = \operatorname{sign}(M\,|\,N\cup P)\operatorname{sign}(P\,|\,N), \tag{2.5b}$$

$$\operatorname{sign}(M\,|\,N) = \begin{cases} 0, & (\text{if } M\cap N \neq \emptyset); \\ \prod\limits_{j=1}^{|N|}(-1)^{|\{\mu\in M\,|\,\mu>\nu_j\}|}, & \textit{with } N=\{\nu_1,\dots,\nu_n\} \textit{ and } \nu_1<\dots<\nu_n; \\ & (\text{if } M\cap N=\emptyset). \end{cases} \tag{2.5c}$$

Let us first consider anticommuting operators:

Lemma 2.2

Let $(A_\mu)_{\mu\in\mathcal{N}}$, $(B_\mu)_{\mu\in\mathcal{N}}$ be families of anticommuting operators, i.e.

$$\{A_\mu, A_\nu\} = \{B_\mu, B_\nu\} = \{A_\mu, B_\nu\} = 0 \quad \text{for all} \quad \mu,\nu\in\mathcal{N}. \tag{2.6}$$

Then for any finite $M, N \subseteq \mathcal{N}$ and for any $\lambda\in\mathbb{C}$ the following relations are valid:

$$A^M A^N = \operatorname{sign}(M\,|\,N) A^{M\cup N}, \tag{2.7a}$$

$$(A+B)^M = \sum_{N\subseteq M}\operatorname{sign}(M\backslash N\,|\,N) A^{M\backslash N} B^N, \tag{2.7b}$$

$$(\lambda A)^M = \lambda^{|M|} A^M, \tag{2.7c}$$

$$(A^M)^+ = (-1)^{\frac{1}{2}|M|(|M|-1)} A^{+M}, \tag{2.7d}$$

$$(AB)^M = (-1)^{\frac{1}{2}|M|(|M|-1)} A^M B^M. \tag{2.7e}$$

Proof: Relation (2.7a) follows immediately from the definition of the signum and from the anticommutation relations. The other rules are proven by induction, for example: (2.7b) is valid for $M=\emptyset$. If it holds for $M=\{\mu_1,\dots,\mu_m\}$ let

$$M' = \{\mu_1,\dots,\mu_m\}\cup\{\mu_{m+1}\}.$$

Then

$$\begin{aligned}(A+B)^{M'} &= (A+B)^M (A_{\mu_{m+1}} + B_{\mu_{m+1}}) \\ &= \sum_{N\subseteq M}\operatorname{sign}(M\backslash N\,|\,N) A^{M\backslash N} B^N \cdot (A_{\mu_{m+1}} + B_{\mu_{m+1}}) \\ &= \sum_{N\subseteq M}(\operatorname{sign}(M\backslash N\,|\,N)(-1)^{|N|} \cdot A^{M'\backslash N} B^N + \operatorname{sign}(M\backslash N\,|\,N) \cdot A^{M'\backslash(N\cup\{\mu_{m+1}\})} B^{N\cup\{\mu_{m+1}\}} \\ &= \sum_{N\subseteq M'}\operatorname{sign}(M'\backslash N\,|\,N) A^{M'\backslash N} B^N. \blacksquare\end{aligned}$$

Similar rules hold for families of commuting operators:

Lemma 2.3

Let the operators of the families $(A_\mu)_{\mu\in\mathcal{N}}$ and $(B_\mu)_{\mu\in\mathcal{N}}$ commute with each other, i.e.

$$[A_\mu, A_\nu] = [B_\mu, B_\nu] = [A_\mu, B_\nu] = 0 \tag{2.8}$$

for all $\mu,\nu\in\mathcal{N}$. Then for any finite subset $M, N\subseteq\mathcal{N}$ and any $\lambda\in\mathbb{C}$ we have

$$(A+B)^M = \sum_{N\subseteq M} A^{M\backslash N} B^N, \tag{2.9b}$$

$$(\lambda A)^M = \lambda^{|M|} A^M, \tag{2.9c}$$

$$(A^M)^+ = A^{+M}, \tag{2.9d}$$

$$(AB)^M = A^M B^M. \tag{2.9e}$$

Proof: In the same way as for Lemma 2.2.

Lemma 2.4. (CAR-families)

Let the operators $(a_\mu)_{\mu\in\mathcal{N}}$ and $(a_\mu^+)_{\mu\in\mathcal{N}}$ fulfill the canonical anticommutation relations

$$\{a_\mu, a_\nu\} = 0, \quad \{a_\mu, a_\nu^+\} = \delta_{\mu\nu} I \quad \textit{for all} \quad \mu,\nu\in\mathcal{N}. \tag{2.10}$$

Then for all finite subsets M, N:

$$a^M a^{+N} = \sum_{Q\subseteq M\cap N}(-1)^{\frac{1}{2}|Q|(|Q|-1)+|M\backslash Q|\,|N\backslash Q|}\operatorname{sign}(M\backslash Q\,|\,Q)\operatorname{sign}(Q\,|\,N\backslash Q)\, a^{+N\backslash Q} a^{M\backslash Q}. \tag{2.11}$$

Proof: For finite $M\subseteq\mathcal{N}$ and $N=\emptyset$ relation (2.11) is trivial. If (2.11) is valid for M and all P with $|P|\leq n$, we can apply the proposition of induction twice and get with

$$N' = \{\nu_1,\nu_2,\dots,\nu_{n+1}\} = \{\nu_1\}\cup\{\nu_2,\dots,\nu_{n+1}\} = \{\nu_1\}\cup N,$$

$$\begin{aligned} a^M a^{+N'} = &\sum_{R\subseteq M\cap\{\nu_1\}}\ \sum_{P\subseteq(M\backslash R)\cap N}(-1)^{\frac{1}{2}|R|(|R|-1)+|M\backslash R|\,|\{\nu_1\}\backslash R|+\frac{1}{2}|P|(|P|-1)+|M\backslash R\backslash P|\,|N\backslash P|} \\ &\cdot\operatorname{sign}(M\backslash R\,|\,R)\operatorname{sign}(R\,|\,\{\nu_1\}\backslash R)\operatorname{sign}(M\backslash R\backslash P\,|\,P)\operatorname{sign}(P\,|\,N\backslash P)\, a^{+\{\nu_1\}\backslash R} a^{+N\backslash P} a^{M\backslash R\backslash P}.\end{aligned} \tag{2.12}$$

In each term of the sum R can only be $\emptyset$ or $\{\nu_1\}$. We put $Q := R\cup P$. As $R\cap P=\emptyset$, we have $|Q| = |R|+|P|$. Then terms with $R=\emptyset$ are

$$(-1)^{|M|+\frac{1}{2}|Q|(|Q|-1)+|M\backslash Q||N'\backslash Q\backslash\{\nu_1\}|}\operatorname{sign}(M\backslash Q\,|\,Q)\operatorname{sign}(Q\,|\,N'\backslash\{\nu_1\}\backslash Q)\,a^{+N'\backslash Q}a^{M\backslash Q}$$
$$=(-1)^{\frac{1}{2}|Q|(|Q|-1)+|M\backslash Q||N'\backslash Q|}(-1)^{|Q|}\operatorname{sign}(M\backslash Q\,|\,Q)(-1)^{|Q|}\operatorname{sign}(Q\,|\,N'\backslash Q)\,a^{+N'\backslash Q}a^{M\backslash Q}, \tag{2.13}$$

while terms with $R=\{\nu_1\}$ are

$$(-1)^{\frac{1}{2}(|Q|-1)(|Q|-2)+|M\backslash Q||N'\backslash Q|}\operatorname{sign}(M\backslash Q\,|\,Q\backslash\{\nu_1\})\operatorname{sign}(M\backslash\{\nu_1\}\,|\,\{\nu_1\})$$
$$\cdot\operatorname{sign}(Q\backslash\{\nu_1\}\,|\,N'\backslash\{\nu_1\}\backslash Q)\,a^{+N'\backslash Q}a^{M\backslash Q}$$
$$=(-1)^{\frac{1}{2}|Q|(|Q|-1)+|M\backslash Q||N'\backslash Q|}(-1)^{|Q|-1}\operatorname{sign}(M\backslash Q\,|\,Q)(-1)^{|Q|-1}\operatorname{sign}(Q\,|\,N\backslash Q)\,a^{+N'\backslash Q}a^{M\backslash Q}. \tag{2.14}$$

All finite subsets $Q\subseteqq M\cap N'$ are included by $Q=R\cup P$ if $R\subseteqq M\cap\{\nu_1\}$ and $P\subseteqq M\cap N$. Therefore, relation (2.11) is also valid for N' and by induction for all $M, N\subseteqq\mathcal{N}$. ∎

If $(a_\mu)_{\mu\in\mathcal{N}}$, $(a_\mu{}^+)_{\mu\in\mathcal{N}}$ and $(b_\mu)_{\mu\in\mathcal{N}}$, $(b_\mu{}^+)_{\mu\in\mathcal{N}}$ are anticommuting CAR-families, the following relations can be deduced by using Lemma 2.2 and Lemma 2.4:

$$a^{+P}a^{M}a^{+N}=\sum_{Q\subseteqq M\cap N}(-1)^{\frac{1}{2}|Q|(|Q|-1)+|M\backslash Q||N\backslash Q|}\operatorname{sign}(M\backslash Q\,|\,Q)\operatorname{sign}(Q\,|\,N\backslash Q)\operatorname{sign}(P\,|\,N\backslash Q)$$
$$\cdot\,a^{+(P\cup(N\backslash Q))}a^{M\backslash Q}, \tag{2.15}$$

$$(b^++a)^{M}a^{+N}=\sum_{P\subseteqq M}\sum_{Q\subseteqq P\cap N}(-1)^{\frac{1}{2}|Q|(|Q|-1)+|P\backslash Q||N\backslash Q|}\operatorname{sign}(M\backslash P\,|\,P)\operatorname{sign}(P\backslash Q\,|\,Q)\operatorname{sign}(Q\,|\,N\backslash Q)$$
$$\cdot\,b^{+M\backslash P}a^{+N\backslash Q}a^{P\backslash Q}. \tag{2.16}$$

If we have in addition a representation of the CAR-algebra with a vector Ω, which is a "vacuum" with respect to the a_μ's, i.e.

$$a_\mu\Omega=0\quad\text{for all}\quad\mu\in\mathcal{N}. \tag{2.17}$$

Then the following identities are valid:

$$a^{M}a^{+N}\Omega=\begin{cases}0, & \text{if}\quad M\nsubseteq N,\\ (-1)^{\frac{1}{2}|M|(|M|-1)}\operatorname{sign}(M\,|\,N\backslash M)\,a^{+N\backslash M}\Omega, & \text{if}\quad M\subseteqq N;\end{cases} \tag{2.18}$$

$$a^{+P}a^{M}a^{+N}\Omega=\begin{cases}0, & \text{if}\quad M\nsubseteq N,\\ (-1)^{\frac{1}{2}|M|(|M|-1)}\operatorname{sign}(M\,|\,N\backslash M)\operatorname{sign}(P\,|\,N\backslash M)\,a^{+(P\cup(N\backslash M))}\Omega, & \text{if}\quad M\subseteqq N;\end{cases} \tag{2.19}$$

$$(b^++a)^{M}a^{+N}\Omega=\sum_{P\subseteqq M\cap N}(-1)^{\frac{1}{2}|P|(|P|-1)}\operatorname{sign}(M\backslash P\,|\,P)\operatorname{sign}(P\,|\,N\backslash P)\,b^{+M\backslash P}a^{+N\backslash P}\Omega. \tag{2.20}$$

Let us introduce the following notation for the frequently occurring operator series (2.3): $(c_\mu)_{\mu\in\mathcal{N}}$ and $(d_\mu)_{\mu\in\mathcal{N}}$ being arbitrary operator families, define

$$h(c,d):=\sum_{\substack{M\subseteqq\mathcal{N}\\ M\text{ finite}}}\sum_{\substack{N\subseteqq\mathcal{N}\\ N\text{ finite}}}h_{MN}\,c^{M}d^{N} \tag{2.21}$$

(not regarding at present any possible convergence problems). Especially for states of the Fock space

$$\Psi=\sum_{\substack{M\subseteqq\mathcal{N}\\ M\text{ finite}}}\psi_M\,a^{+M}\Omega$$

we introduce the operator

$$\psi(b):=\sum_{\substack{M\subseteqq\mathcal{N}\\ M\text{ finite}}}\psi_M\,b^{M}, \tag{2.22}$$

which in the case $b_\mu=a_\mu{}^+$ can be taken for the "creation" operator of the state vector Ψ.

We want to define the "inner product" of two operator families $A=(A_\mu)_{\mu\in M}$, $B=(B_\mu)_{\mu\in M}$ (M finite subset of $\mathcal{N}$) by the operator

$$A\cdot B:=\sum_{\mu\in M}A_\mu B_\mu. \tag{2.23}$$

The following lemma is known as the Baker-Hausdorff formula:

Lemma 2.5

For a finite subset $M\subseteqq\mathcal{N}$ let $(a_\mu)_{\mu\in M}$, $(a_\mu{}^+)_{\mu\in M}$ be CAR-families and $(b_\mu{}^+)_{\mu\in\mathcal{N}}$ another family anticommuting with $(a_\mu)_{\mu\in M}$, $(a_\mu{}^+)_{\mu\in M}$. Then for the operator of the (finite) series

$$e^{ia^+\cdot b^+}:=\sum_{k=0}^{\infty}\frac{1}{k!}\,i^k(a^+\cdot b^+)^k \tag{2.24}$$

and every $\nu\in M$

$$e^{ia^+\cdot b^+}a_\nu e^{-ia^+\cdot b^+}=a_\nu-ib_\nu{}^+. \tag{2.25}$$

Proof: Let $F(\lambda)$ be the operator-valued, differentiable function

$$F(\lambda) := e^{i\lambda a^+ \cdot b^+} a_\nu e^{-i\lambda a^+ \cdot b^+}$$

with the real parameter $\lambda \in \mathbb{R}$. Its derivative with respect to λ is

$$\left(\frac{\mathrm{d}}{\mathrm{d}\lambda} F\right)(\lambda) = e^{i\lambda a^+ \cdot b^+}(i a^+ \cdot b^+ a_\nu - i a_\nu a^+ \cdot b^+) \cdot e^{-i\lambda a^+ \cdot b^+} = - i b_\nu^+ . \quad (2.26)$$

This ordinary differential equation with the initial condition $F(0) = a_\nu$ has the unique solution

$$F(\lambda) = a_\nu - \lambda i b_\nu^+ . \quad (2.27)$$

Putting $\lambda = 1$ leads to the assertion. ▮

Let us finally note the following: If $(a_\nu)_{\nu \in \mathcal{N}}$, $(a_\nu^+)_{\nu \in \mathcal{N}}$, $(b_\nu)_{\nu \in \mathcal{N}}$, $(b_\nu^+)_{\nu \in \mathcal{N}}$ are anticommuting CAR-families and Ω is a vector of a representation of $\mathfrak{A}$ with $a_\nu \Omega = 0$ for all $\nu \in \mathcal{N}$, then for all operator functions $h(b^+, b)$:

$$\underbrace{a_\nu h(b^+, b)}_{\llcorner\_\_\_\_\uparrow} \Omega = 0 . \quad (2.28)$$

In each term of $h(b^+, b)$, a_ν can be brought in front of Ω to give 0, and factors (-1) from commutations are irrelevant.

§ 3. The CAR Tensor Product

Let $\mathscr{C}_a$ and $\mathscr{C}_b$ be one-particle Hilbert spaces with complete orthonormal systems $(w_\nu)_{\nu \in \mathscr{V}}$ and $(r_\lambda)_{\lambda \in \mathscr{L}}$ respectively; e.g. $\mathscr{C}_a$ can stand for the set of one-particle states of the valence band (with index set $\mathscr{V} \subseteqq \mathcal{N}$) and $\mathscr{C}_b$ can stand for the set of conduction band states (with index set $\mathscr{L} \subseteqq \mathcal{N}$). If the one-particle system can choose between any of the states in $\mathscr{C}_a$ or $\mathscr{C}_b$, we describe the system by $\mathscr{C} = \mathscr{C}_a \oplus \mathscr{C}_b$ with the complete orthonormal system

$$(s_\mu)_{\mu \in \mathscr{V} \cup \mathscr{L}} = (w_1, \ldots, r_1 \ldots) .$$

We denote by $\mathfrak{A}_a$, $\mathfrak{A}_b$ and $\mathfrak{A}$ the CAR-algebras associated with $\mathscr{C}_a$, $\mathscr{C}_b$ and $\mathscr{C}$ respectively, as constructed in § 1. The corresponding creation and annihilation operators are $(a_\nu^+)_{\nu \in \mathscr{V}}$, $(a_\nu)_{\nu \in \mathscr{V}}$ for the $(w_\nu)_{\nu \in \mathscr{V}}$, $(b_\lambda^+)_{\lambda \in \mathscr{L}}$, $(b_\lambda)_{\lambda \in \mathscr{L}}$ for the $(r_\lambda)_{\lambda \in \mathscr{L}}$, and $(c_\mu^+)_{\mu \in \mathcal{N}}$, $(c_\mu)_{\mu \in \mathcal{N}}$ for the $(s_\mu)_{\mu \in \mathscr{V} \cup \mathscr{L}}$.

The algebra for the joint measurement of observables of $\mathfrak{A}_a$ and $\mathfrak{A}_b$ is called the CAR-tensor product $\mathfrak{A}_a \hat{\otimes} \mathfrak{A}_b$ and is given by the following definition:

Definition 3.1

$\mathfrak{A}_a \hat{\otimes} \mathfrak{A}_b$ is called a CAR-tensor product of $\mathfrak{A}_a$ and $\mathfrak{A}_b$, iff there are mappings

$$f_a\colon \mathfrak{A}_a \to \mathfrak{A}_a \hat{\otimes} \mathfrak{A}_b , \quad (3.1)$$

$$f_b\colon \mathfrak{A}_b \to \mathfrak{A}_a \hat{\otimes} \mathfrak{A}_b \quad (3.2)$$

with the properties

(i) *f_a and f_b are linear, multiplicative, isometric, and*

$$f_a(A^+) = f_a(A)^+ , \quad f_b(B^+) = f_b(B)^+ \quad \text{for all} \quad A \in \mathfrak{A}_a , \quad B \in \mathfrak{A}_b . \quad (3.3)$$

(ii) *The images of the CAR-operators under the mappings f_a and f_b are anticommuting families:*

$$\{f_a(a_\nu), f_b(b_\lambda)\} = \{f_a(a_\nu), f_b(b_\lambda^+)\} = 0; \quad \nu \in \mathscr{V}, \quad \lambda \in \mathscr{L}. \quad (3.4)$$

(iii) *The images of the CAR-operators a_ν, a_ν^+ under f_a and b_λ, b_λ^+ under f_b generate the CAR-tensor product:*

$$\mathfrak{A}_a \hat{\otimes} \mathfrak{A}_b = \text{norm-completion} \cdot \langle \{f_a(a_\nu), f_a(a_\nu^+), f_b(b_\lambda), f_b(b_\lambda^+) \mid \nu \in \mathscr{V}, \lambda \in \mathscr{L}\} \cup \{\mathrm{I}\} \rangle . \quad (3.5)$$

(iv) *The norm on $\mathfrak{A}_a \hat{\otimes} \mathfrak{A}_b$ is identical with the operator norm in every tensor product of representations.*

With this definition we get the existence and uniqueness of the CAR-tensor product algebra:

Theorem 3.2

The CAR-tensor product of the CAR-algebras $\mathfrak{A}_a$ and $\mathfrak{A}_b$ is given by

$$\mathfrak{A}_a \hat{\otimes} \mathfrak{A}_b = \mathfrak{A} , \quad (3.6)$$

with $\mathfrak{A}$ being the CAR-algebra associated with $\mathscr{C} := \mathscr{C}_a \oplus \mathscr{C}_b$.

Proof: Using the notations as above we define:

$$f_a(a_\nu) := c_\nu , \quad f_a(a_\nu^+) := c_\nu^+ , \quad f_a(I_{\mathfrak{A}_a}) = I_{\mathfrak{A}} \quad (\nu \in \mathscr{V}); \quad (3.7)$$

$$f_b(b_\lambda) := c_\lambda , \quad f_b(b_\lambda^+) := c_\lambda^+ , \quad f_b(I_{\mathfrak{A}_b}) = I_{\mathfrak{A}} \quad (\lambda \in \mathscr{L}) . \quad (3.8)$$

These transformations can be uniquely extended to multiplicative and linear transformations on $\mathfrak{A}_a$, respectively $\mathfrak{A}_b$. Then f_a and f_b fulfill all conditions of Def. 3.1. Conversely, given an algebra $\mathfrak{B}$ fulfilling all conditions of Def. 3.1, we define an isomorphism f from $\mathfrak{B}$ to $\mathfrak{A}$ by the linear and continuous extension of

$$f(f_a(a_\nu)) := c_\nu, \quad f(f_a(a_\nu^+)) := c_\nu^+ \quad (\nu \in \mathscr{V});$$
$$f(f_b(b_\lambda)) = c_\lambda, \quad f(f_b(b_\lambda^+)) = c_\lambda^+ \quad (\lambda \in \mathscr{L})$$

and $f(I_{\mathfrak{B}}) = I_{\mathfrak{A}}$. Thus $\mathfrak{B}$ and $\mathfrak{A}$ are isomorphic. ▮▮

Remark: From here on we will disregard the difference between the image and inverse image of the embedding isomorphisms f_a and f_b and simply identify

$$a_\nu \equiv f_a(a_\nu) = c_\nu \quad (\nu \in \mathscr{V}), \tag{3.9}$$

$$b_\lambda \equiv f_b(b_\lambda) = c_\lambda \quad (\lambda \in \mathscr{L}). \tag{3.10}$$

Now consider the Fock space representation on $\mathscr{H}_{\Omega_a}$ of the algebra $\mathfrak{A}_a$ corresponding to the cyclic vector Ω_a and another arbitrary IDPS representation on $\mathscr{H}_{\Psi_b}$ of $\mathfrak{A}_b$ corresponding to the reference vector Ψ_b. Then the CAR-tensor product algebra $\mathfrak{A}_a \hat{\otimes} \mathfrak{A}_b$ can be represented canonically on

$$\mathscr{H}_{\Omega_a} \otimes \mathscr{H}_{\Psi_b} = \mathscr{H}_{\Omega_a \otimes \Psi_b}$$

with cyclic vector $\Omega_a \otimes \Psi_b$ by defining

$$(A \hat{\otimes} B)(\chi_a \otimes \chi_b) := A\chi_a \otimes B\chi_b .$$

Let $\chi \in \mathscr{H}_{\Psi_b}$ and

$$A = \sum_{K,L \subsetneq \mathscr{V}} \alpha_{KL}\, a^{+K} a^L \in \mathfrak{A}_a ,$$
$$B = \sum_{M,N \subsetneq \mathscr{L}} \beta_{MN}\, b^{+M} b^N \in \mathfrak{A}_b .$$

Then

$$\begin{aligned} A\Omega_a \otimes B\chi &= \sum_{K,L \subsetneq \mathscr{V}} \sum_{M,N \subsetneq \mathscr{L}} \alpha_{KL} \beta_{MN}\, \Omega_a \otimes b^{+M} b^N \chi \\ &= \sum_{K,L \subsetneq \mathscr{V}} \sum_{M,N \subsetneq \mathscr{L}} \alpha_{KL}\, a^{+K} a^L \beta_{MN} \\ &\quad \cdot b^{+M} b^N \Omega_a \otimes \chi \\ &= AB(\Omega_a \otimes \chi), \end{aligned} \tag{3.11}$$

where we have used the identification mentioned in the remark above.

§ 4. A Conjugation on Hilbert Space and its Properties

In II it will turn out that the New-Tamm-Dancoff system is equivalent to an eigenvalue equation of the tensor product of the Hamiltonian with a Hamiltonian conjugate to the original one. Here we want to treat some aspects of the conjugation. As is well known, conjugations are characterized by the following

Definition 4.1

Let $\mathscr{H}$ be a Hilbert space.

a) *A mapping $\triangle$: $\mathscr{H} \to \mathscr{H}$, $\Psi \mapsto \Psi^\triangle$ is called a (continuous) conjugation, if $\triangle$ is antilinear, involutoric, and isometric:*

$$(\alpha\Psi + \beta\chi)^\triangle = \bar{\alpha}\Psi^\triangle + \bar{\beta}\chi^\triangle ,$$
$$\Psi^{\triangle\triangle} = \Psi, \quad \|\Psi^\triangle\| = \|\Psi\| . \tag{4.1}$$

b) *If $\triangle$ is a conjugation and A is an operator with domain $\mathscr{D}(A)$ in $\mathscr{H}$, we define*

$$\mathscr{D}(A^\triangle) := \mathscr{D}(A)^\triangle \quad \text{and}$$
$$A^\triangle \Psi^\triangle := (A\Psi)^\triangle \quad \text{for all} \quad \Psi \in \mathscr{D}(A). \tag{4.2}$$

The following elementary properties of a conjugation are easily verified:

$$\langle \Psi^\triangle | \chi^\triangle \rangle = \overline{\langle \Psi | \chi \rangle} \tag{4.3}$$

(use the polarisation identity)

$$(\alpha A + \beta B)^\triangle = \bar{\alpha} A^\triangle + \bar{\beta} B^\triangle , \tag{4.4}$$

$$(AB)^\triangle = A^\triangle B^\triangle \tag{4.5}$$

(no interchange of factors!)

$$I^\triangle = I . \tag{4.6}$$

The following theorem is important for the physical interpretation of the conjugate operator:

Theorem 4.2

If A is a selfadjoint operator with the spectral resolution $(E(\lambda))_{\lambda \in \mathbb{R}}$, then $A^\triangle$ is also selfadjoint and its spectral resolution is $(E(\lambda)^\triangle)_{\lambda \in \mathbb{R}}$.

Proof: $A^\triangle$ is uniquely determined by the values of the sesquilinear form

$$\langle \Psi^\triangle A^\triangle \chi^\triangle \rangle \quad \text{with} \quad \Psi, \chi \in \mathscr{D}(A).$$

We have

$$\begin{aligned} \langle \Psi^\triangle | A^\triangle \chi^\triangle \rangle &= \langle \Psi^\triangle | (A\chi)^\triangle \rangle = \langle A\chi | \Psi \rangle \\ &\underset{\substack{\text{spectral}\\ \text{theorem}}}{=} \int \lambda \,\mathrm{d}\langle E(\lambda)\chi | \Psi \rangle \\ &= \int \lambda \,\mathrm{d}\langle \Psi^\triangle | (E(\lambda)\chi)^\triangle \rangle . \end{aligned} \tag{4.7}$$

Further, for $\Psi \in \mathscr{H}$

$$\lim_{\lambda \to \infty} E(\lambda)^\triangle \Psi^\triangle = \lim_{\lambda \to \infty} (E(\lambda)\Psi)^\triangle = \Psi^\triangle , \tag{4.8}$$

and, the same way

$$\lim_{\lambda \to -\infty} E(\lambda)^\triangle \Psi^\triangle = 0 . \tag{4.9}$$

We further have

$$E(\lambda)^{\triangle} E(\mu)^{\triangle} = (E(\lambda) E(\mu))^{\triangle} = E(\lambda)^{\triangle} \quad \text{if} \quad \lambda \leqq \mu . \tag{4.10}$$

The properties (4.7)—(4.10) uniquely characterize the spectral resolution of $A^{\triangle}$, see e.g. [8], p. 170 (7.11) and p. 181 (7.17). Therefore $A^{\triangle}$ is selfadjoint with spectral resolution $(E(\lambda)^{\triangle})_{\lambda \in \mathbb{R}}$. ▮▮

This theorem expresses the spectral properties of A and $A^{\triangle}$ being the same. So we can investigate the properties of $A^{\triangle}$ instead of A to get the same physical interpretation.

In the New-Tamm-Dancoff procedure (see II) a mapping $\Psi \mapsto \Psi^{\triangle}$ occurs with $\Psi^{\triangle} = \psi(ia)^{+}\Omega$ for $\Psi = \psi(a^{+})\Omega \in \mathscr{H}_{\Omega}(\mathscr{C})$. Here we prepare the most important formulae for this mapping:

Lemma 4.3

The mapping $\psi(a^{+})\Omega \mapsto \psi(ia)^{+}\Omega$ is a conjugation on the Fock space. The following relations hold

$$\Psi^{\triangle} = \sum_{M \subsetneqq \mathscr{N}} (-1)^{\frac{1}{2}|M|(|M|-1)} \cdot \overline{\psi}_M (-i)^{|M|} a^{+M} \Omega , \tag{4.11}$$

$$a_{\mu}^{+\triangle} = (-i a_{\mu}^{+})(-1)^{\mathscr{Z}} , \tag{4.12}$$

$$a_{\mu}^{\triangle} = (-i a_{\mu})(-1)^{\mathscr{Z}} , \tag{4.13}$$

$$(a^{+M} a^{N})^{\triangle} = a^{+M} a^{N} , \quad \textit{if} \quad |M| + |N| \ \textit{is even}. \tag{4.14}$$

Here the sign-operator $(-1)^{\mathscr{Z}}$ is given by

$$(-1)^{\mathscr{Z}} a^{+M} \Omega = (-1)^{|M|} a^{+M} \Omega . \tag{4.15}$$

Proof: Obviously $\triangle$ is antilinear. For a finite sum of basis vectors of the Fock space we have

$$\Psi^{\triangle} = \Big(\sum_{M \subsetneqq \mathscr{N}} \psi_M (ia)^M \Big)^{+} \Omega = \sum_{M \subsetneqq \mathscr{N}} \overline{\psi}_M (-i)^{|M|} (-1)^{\frac{1}{2}|M|(|M|-1)} a^{+M} \Omega . \tag{4.16}$$

On these elements $\triangle$ is isometric, therefore $\triangle$ is isometric on $\mathscr{H}_{\Omega}(\mathscr{C})$ at all. By use of (4.16) it is easily verified that $\triangle$ is involutoric.

Let us prove (4.12). It is sufficient to show, that the relation holds if applied to all elements $(a^{+M}\Omega)^{\triangle}$

$$\begin{aligned} a_{\mu}^{+\triangle}(a^{+M}\Omega)^{\triangle} &= (a_{\mu}^{+} a^{+M}\Omega)^{\triangle} \\ &= (-1)^{\frac{1}{2}(|M|+1)|M|} (-i)^{|M|+1} a_{\mu}^{+} a^{+M} \Omega \\ &= (-1)^{\frac{1}{2}(|M|+1)|M|} (-i)^{|M|+1} (-1)^{\frac{1}{2}|M|(|M|-1)} \cdot i^{|M|} a_{\mu}^{+} (a^{+M}\Omega)^{\triangle} \\ &= (-i a_{\mu}^{+})(-1)^{\mathscr{Z}} (a^{+M}\Omega)^{\triangle} . \end{aligned}$$

Analoguously (4.13) is shown. With these results we get

$$(a^{+M} a^{N})^{\triangle} = (-i a^{+})^{M} (-i a)^{N} \cdot (-1)^{\frac{1}{2}(|M|+|N|)(|M|+|N|-1)} \cdot (-1)^{(|M|+|N|)\mathscr{Z}} ,$$

so especially for $|M| + |N|$ even

$$(a^{+M} a^{N})^{\triangle} = a^{+M} a^{N} . \quad ▮▮$$

An immediate consequence of this is: The operator

$$H = \sum_{\substack{M, N \subsetneqq \mathscr{N} \\ |M|+|N| \text{ even}}} h_{MN} a^{+M} a^{N} = h(a^{+}, a)$$

has the conjugate

$$H^{\triangle} = \sum_{\substack{M, N \subsetneqq \mathscr{N} \\ |M|+|N| \text{ even}}} \overline{h}_{MN} a^{+M} a^{N} =: h^{\triangle}(a^{+}, a) . \tag{4.17}$$

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