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

II. Functional Quantum Mechanics and the Equivalence with a Product of Schrödinger Problems

F. Wahl and W. Feist

Universität Tübingen, Institut für Theoretische Physik, Tübingen

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The New Tamm-Dancoff procedure consists of three main parts: an expansion for pairs of states with respect to a non-orthogonal base, a cut-off approximation for this expansion, and a transformation with respect to a new reference state. In this paper we treat part one and two. It is shown that the NTD-procedure is equivalent to the tensor product of the original Schrödinger problem and its conjugate problem. The occurring nonlinear transformation is examined and the cut-off is discussed.

§ 5. Introduction

Tamm [1] and Dancoff [2] independently introduced a procedure for the approximative determination of eigenvalues in quantum field theory. It is based on an expansion with respect to a complete orthonormal system in Fock space with a cut off at finite order. To avoid certain divergences of principal nature, Dyson [3] proposed a modification, the so-called New-Tamm-Dancoff procedure (NTD-procedure). Instead of a single eigenstate in Fock space a pair of states is expanded with respect to coordinates (as will be shown in § 11 nonorthogonal ones) and this expansion is cut off at finite order. Following Heisenberg [4], many of his former students applied this procedure to a great extend, especially Stumpf [5], Dürr and Wagner [6].

The convergence was proved in the case of the anharmonic oscillator in [7]. On account of considerable mathematical difficulties in relativistic quantum field theory, the procedure was first tested in solid state theory [8]. It turned out that it has advantages in calculating approximations for complicated many body systems [9].

This work classifies the NTD-procedure in the mathematical framework of the algebraic theory of many body systems [10, 11]. As a guidance the treatment of electrons and holes in a semiconductor was used, but any nonrelativistic solid state problem may be treated in a similar way.

Reprint requests to Prof. Dr. F. Wahl, Institut für Theoretische Physik, Universität Tübingen, Auf der Morgenstelle, D-7400 Tübingen.

The notation is the same as in [13], which will be abbreviated by I in the following. Only local systems with an energy cut off will be considered. As in I let $(w_\nu)_{\nu\in\mathcal{N}}$ be an orthonormal base of vectors in the finite dimensional one-particle Hilbert space $\mathcal{C}$. The families of creation- and annihilation operators with respect to this base are denoted by $(a_\nu^+)_{\nu\in\mathcal{N}}$ and $(a_\nu)_{\nu\in\mathcal{N}}$, respectively. Let the local Hamiltonian (with energy cut off) be

$$H = h(a^+, a) = \sum_{M,N\subseteq\mathcal{N}} h_{MN}\, a^{+M} a^N . \tag{5.1}$$

To specify examples, the expressions [8, (1.13)] and [9, (2.1)] are of this type. We suppose H to be self-adjoint, i.e.

$$h_{MN} = \bar{h}_{NM}(-1)^{\frac{1}{2}|M|(|M|-1)+\frac{1}{2}|N|(|N|-1)} . \tag{5.2}$$

The NTD-procedure consists of three main parts:

(i) The *pairs of states are expanded* with respect to a certain (non-orthogonal) basis, and the eigenvalue problem is transformed into a matrix equation for the coefficients of this expansion. As will be shown, the system is equivalent to the direct product of the Schrödinger problem and its conjugate under a non-unitary transformation [§ 6–§ 10].

(ii) The resulting system of equations is *truncated* [§ 12]. The various approximations are discussed in [8] for a solid state model.

(iii) As the ground state of a semiconductor model is characterized by a completely filled valence band, the analysis shown in §§ 6 to 12 is not done in the Fock space representation cor-

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responding to the pure vacuum, but in the *valence band representation*. Within the NTD-formalism this is accomplished by the F-transformation (see [14], which will be abbreviated by III in the following).

§ 6. Determination of Energy Differences; the φ-coefficients

In many body physics the ground state energy in many cases is very large compared with the energy difference between neighbouring states. In the thermodynamic limit only energy differences with respect to a reference-state are important. For a method to determine such energy difference (introduced by Dyson [3] and Freese [19]) we state

Theorem 6.1

Two state vectors Ψ *and* χ ($\|\Psi\| = \|\chi\| = 1$) *of the Fock space are both eigenvectors of* H *if and only if*

$$\langle\Psi|(HA - AH)\chi\rangle = \omega_{\Psi\chi}\langle\Psi|A\chi\rangle . \tag{6.1}$$

holds for all $A \in L(\mathscr{H}_\Omega)$. *The eigenvalues are related by*

$$\omega_{\Psi\chi} = \varepsilon_\Psi - \varepsilon_\chi . \tag{6.2}$$

Proof: For eigenstates Ψ and χ we have $H\Psi = \varepsilon_\Psi\Psi$ and $H\chi = \varepsilon_\chi\chi$. Thus

$$\begin{aligned}\langle\Psi|(HA - AH)\chi\rangle &= \langle H\Psi|A\chi\rangle \\ &\quad - \langle\Psi|AH\chi\rangle \\ &= (\varepsilon_\Psi - \varepsilon_\chi)\langle\Psi|A\chi\rangle .\end{aligned}$$

To prove the converse, let (6.1) be valid for all $A \in L(\mathscr{H}_\Omega)$. Let Ψ', χ' be arbitrary vectors in $\mathscr{H}_\Omega$ and $A_{\Psi'\chi'}$ the operator

$$A_{\Psi'\chi'}(\Phi) := \Psi'\langle\chi'|\Phi\rangle \quad (\Phi \in \mathscr{H}_\Omega) . \tag{6.3}$$

We then have for all $\Psi' \in \mathscr{H}_\Omega$ with $\|\Psi'\| = 1$

$$\begin{aligned}|\langle\Psi|[H, A_{\Psi\chi}]\chi\rangle| &= |\omega_{\Psi\chi}\langle\Psi|\Psi\rangle\langle\chi|\chi\rangle| \\ &\geqq |\omega_{\Psi\chi}||\langle\Psi|\Psi'\rangle||\langle\chi|\chi\rangle| \\ &= |\langle\Psi|[H, A_{\Psi'\chi}]\chi\rangle| .\end{aligned}$$

Thus

$$\begin{aligned}&|\langle\Psi|[H, A_{\Psi\chi}]\chi\rangle| \\ &= \sup_{\|\Psi'\|=1} |\langle\Psi|[H, A_{\Psi'\chi}]\chi\rangle| .\end{aligned} \tag{6.4}$$

Let $\varepsilon_\chi := \langle\chi|H\chi\rangle$, so we get

$$\begin{aligned}|\langle\Psi|[H, A_{\Psi'\chi}]\chi\rangle &= \langle\Psi|(H\Psi'\langle\chi|\chi\rangle \\ &\quad - \Psi'\langle\chi|H\chi\rangle)\rangle \\ &= \langle(H - \varepsilon_\chi)\Psi|\Psi'\rangle\end{aligned} \tag{6.5}$$

(6.4) and (6.5) yield

$$\begin{aligned}&|\langle(H - \varepsilon_\chi)\Psi|\Psi\rangle|^2 = |\langle\Psi|[H, A_{\Psi\chi}]\chi\rangle|^2 \\ &= \sup_{\|\Psi'\|=1} |\langle\Psi|[H, A_{\Psi'\chi}]\chi\rangle|^2 \\ &= \sup_{\|\Psi'\|=1} |\langle(H - \varepsilon_\chi)\Psi|\Psi'\rangle|^2 \\ &= \|(H - \varepsilon_\chi)\Psi\|^2 .\end{aligned}$$

Riesz

Thus the vectors $(H - \varepsilon_\chi)\Psi$ and Ψ give rise to equality in Cauchy-Schwarz inequality. So they are linear dependent, there is a $\lambda \in \mathbb{C}$ such that

$$(H - \varepsilon_\chi)\Psi = \lambda\Psi .$$

Thus Ψ is an eigenvector of H with the corresponding eigenvalue $\langle\Psi|H\Psi\rangle$. Following the same arguments we show that χ is an eigenvector of H with eigenvalue $\langle\chi|H\chi\rangle$. By the first part of the proof $\omega_{\Psi\chi} = \varepsilon_\Psi - \varepsilon_\chi$. ∎

In the present case with a finite number of degrees of freedom the operators $a^{+M}a^N$ ($M, N \subseteqq \mathscr{N}$) span the algebra $L(\mathscr{H}_\Omega)$. Thus the validity of (6.1) for all $A \in L(\mathscr{H}_\Omega)$ is equivalent to the validity of (6.1) for all A of the form $a^{+M}a^N$. The values of $\langle\Psi|a^{+M}a^N\chi\rangle$ ($M, N \subseteqq \mathscr{N}$) are in a one to one correspondence to the pair of state vectors (Ψ, χ) except form a common phase factor. Slightly deviating we define:

Definition 6.2

Let the φ*-coefficients of the pair of state vectors* (Ψ, χ) *be*

$$\begin{aligned}\varphi_{\Psi\chi}(M|N) &:= i^{|M|+|N|}(-1)^{|M||N|} \\ &\quad \cdot\langle(-1)^{(|M|+|N|)\mathscr{Z}}\Psi|a^{+M}a^N\chi\rangle .\end{aligned} \tag{6.6}$$

($\mathscr{Z}$ is the number operator defined in (I.1)).

Since the $a^{+M}a^N$ form a basis of the algebra $L(\mathscr{H}_\Omega)$, equation (6.1) can be rewritten in terms of the φ-coefficients. This socalled Φ-system will be set up in § 10.

§ 7. The Generating Operator and the Φ-functional

We want to comprehend the φ-coefficients as a vector. This is achieved by defining $\mathfrak{A}_a$, $\mathfrak{A}_u$, $\mathfrak{A}_v$ to be CAR-algebras over the same one-particle Hilbert space $\mathscr{C}$ with corresponding annihilation operators $(a_\nu)_{\nu\in\mathcal{N}}$, $(u_\nu)_{\nu\in\mathcal{N}}$ and $(v_\nu)_{\nu\in\mathcal{N}}$, respectively. We will interprete the a_ν as annihilation operators of the many particle system as usually, but the u_ν and v_ν

as test operators. As in I § 3 the CAR tensor product $\mathfrak{A} := \mathfrak{A}_a \hat{\otimes} \mathfrak{A}_u \hat{\otimes} \mathfrak{A}_v$ is formed and the creation and annihilation operators are identically embedded by $a_\mu^+, a_\mu, u_\mu^+, u_\mu, v_\mu^+, v_\mu$ ($\mu \in \mathcal{N}$). All these operators anticommute except the canonical anticommutation relations

$$\{a_\mu, a_\nu^+\} = \{u_\mu, u_\nu^+\} = \{v_\mu, v_\nu^+\} = \delta_{\mu\nu} I . \quad (7.1)$$

We consider the Fock space representation for each algebra and choose for $\mathfrak{A}$ the product representation on $\mathscr{H}_\Omega(\mathscr{C} \oplus \mathscr{C} \oplus \mathscr{C})$. On this space we define the *generating operator*

$$V := e^{iu^+ \cdot a^+} e^{iv^+ \cdot a} \quad (7.2)$$

(here is $u^+ \cdot a^+ := \sum_{\mu \in \mathcal{N}} u_\mu^+ a_\mu^+$ according to I § 2, (2.23)). This operator series is finite, as $\mathfrak{A}$ is of finite dimension. In the case of infinite degrees of freedom we must restrict the test-space to define V.

Using the calculations in I § 2 the series can be determined:

$$V = \sum_{K, L \subseteq \mathcal{N}} i^{|K|+|L|} (-1)^{\frac{1}{2}(|K|+|L|)(|K|+|L|+1)} \cdot u^{+K} v^{+L} a^{+K} a^L . \quad (7.3)$$

This displays the generating operator comprising all operators $a^{+K} a^L$ ($K, L \subseteq \mathcal{N}$) labelled with coefficient operators $u^{+K} v^{+L}$, respectively.

Now let Ψ and χ be normed vectors in $\mathscr{H}_{\Omega_a}(\mathscr{C})$. We define an antilinear functional on the test space $\mathscr{H}_{\Omega_{uv}}(\mathscr{C} \oplus \mathscr{C})$ corresponding to the pair of states (Ψ, χ). Using the generating operator we associate with each $\Phi' \in \mathscr{H}_{\Omega_{uv}}(\mathscr{C} \oplus \mathscr{C})$ the value

$$\langle \Psi \hat{\otimes} \Phi' \,|\, V(\chi \hat{\otimes} \Omega_{uv}) \rangle ; \quad (7.4)$$

Ω_{uv} denotes the vacuum vector in test space.

We exploit this antilinear functional on the special elements $\Phi' = u^{+M} v^{+N} \Omega_{uv}$ and obtain

$$\begin{aligned}
&\langle \Psi \hat{\otimes} u^{+M} v^{+N} \Omega_{uv} \,|\, V(\chi \hat{\otimes} \Omega_{uv}) \rangle \\
&= \langle \psi(a^+)\, u^{+M} v^{+N} \Omega_{uv} \,|\, V \chi(a^+) \Omega \rangle \\
&= \langle (-1)^{(|M|+|N|)\mathscr{Z}} \psi(a^+) \Omega \,| \\
&\quad \cdot (-1)^{\frac{1}{2}|N|(|N|-1)+\frac{1}{2}|M|(|M|-1)} v^N u^M \\
&\quad \cdot \sum_{K, L \subseteq \mathcal{N}} i^{|K|+|L|} (-1)^{\frac{1}{2}(|K|+|L|)(|K|+|L|-1)} \\
&\quad \cdot u^{+K} v^{+L} a^{+K} a^L \chi(a^+) \Omega \rangle \\
&= i^{|M|+|N|} (-1)^{|M||N|} \\
&\quad \cdot \langle (-1)^{(|M|+|N|)\mathscr{Z}} \Psi \,|\, a^{+M} a^N \chi \rangle \\
&= \varphi_{\Psi\chi}(M \,|\, N) . \quad (7.5)
\end{aligned}$$

Therefore, the antilinear functional defined in (7.4) is called the Φ-functional. As it is defined on a finite dimensional Hilbert space and therefore is continuous, by the Riesz lemma there is a unique element Φ of Hilbert space, such that the Φ-functional is the scalar product

$$\langle \Phi' \,|\, \Phi \rangle := \langle \Psi \hat{\otimes} \Phi' \,|\, V(\chi \hat{\otimes} \Omega_{uv}) \rangle . \quad (7.6)$$

If we want to emphasize the dependence of Φ on the pair of states (Ψ, χ) we write $\Phi = \Phi_{\Psi\chi}$. The set

$$\{\Phi_{\Psi\chi} \,|\, \Psi, \chi \in \mathscr{H}_{\Omega_a}(\mathscr{C})\}$$

is called the functional space $\mathscr{F}$. In the finite dimensional case it is identical to the testspace $\mathscr{H}_{\Omega_{uv}}(\mathscr{C} \oplus \mathscr{C})$. According to (7.5) and (7.6) the expansion of the Φ-functional with respect to the basis $(u^{+M} v^{+N} \Omega_{uv})_{M, N \subseteq \mathcal{N}}$ is

$$\Phi_{\Psi\chi} = \sum_{M, N \subseteq \mathcal{N}} u^{+M} v^{+N} \Omega\, \varphi(M \,|\, N) . \quad (7.7)$$

As intended $\Phi_{\Psi\chi}$ comprehends all φ-coefficients of the pair of states, thus forming a vector of the functional space.

§ 8. Functional Quantum Mechanics

Let us express both sides of (6.1) by the φ-coefficients. The result is a linear eigenvalue equation equivalent to the Schrödinger eigenvalue problem by means of Theorem 6.1. For a detailed analysis we contract (6.1) for all $A = a^{+M} a^N$ to give an eigenvalue equation for the Φ-functional

$$\begin{aligned}
&\langle \Psi \hat{\otimes} \Phi' \,|\, [H, V](\chi \hat{\otimes} \Omega_{uv}) \rangle \\
&= \omega_{\Psi\chi} \langle \Psi \hat{\otimes} \Phi' \,|\, \chi \hat{\otimes} \Omega_{uv} \rangle ,
\end{aligned}$$

tested on all $\Phi' \in \mathscr{H}_{\Omega_{uv}}$. The left-hand side is

$$\begin{aligned}
&\langle \Psi \hat{\otimes} \Phi' \,|\, [H, V](\chi \hat{\otimes} \Omega_{uv}) \rangle \\
&\quad = \langle \Psi \hat{\otimes} \Phi' \,|\, HV(\chi \hat{\otimes} \Omega_{uv}) \rangle \\
&\qquad - \langle \Psi \hat{\otimes} \Phi' \,|\, VH(\chi \hat{\otimes} \Omega_{uv}) \rangle \\
&\quad = \langle (H\Psi) \hat{\otimes} \Phi' \,|\, V(\chi \hat{\otimes} \Omega_{uv}) \rangle \\
&\qquad - \langle \Psi \hat{\otimes} \Phi' \,|\, V(H\chi \hat{\otimes} \Omega_{uv}) \rangle \\
&\quad = \langle \Phi' \,|\, \Phi_{(H\Psi)\chi} - \Phi_{\Psi(H\chi)} \rangle ,
\end{aligned}$$

the right-hand side equals $\omega_{\Psi\chi} \langle \Phi' \,|\, \Phi_{\Psi\chi} \rangle$. Therefore, the equation for the Φ-functional is

$$\Phi_{(H\Psi)\chi} - \Phi_{\Psi(H\chi)} = \omega_{\Psi\chi} \Phi_{\Psi\chi} . \quad (8.1)$$

If we define the functional Hamiltonian by

$$B\Phi_{\Psi\chi} := \Phi_{(H\Psi)\chi} - \Phi_{\Psi(H\chi)} \tag{8.2}$$

the φ-system takes the form

$$B\Phi = \omega\Phi\,. \tag{8.3}$$

Summarizing we have the following statement:

Using the functional formulation of quantum mechanics, we assign an antilinear functional to every pair of states in Fock space. The solution of the eigenvalue problem for a Hamiltonian H in Fock space is equivalent to the solution of the eigenvalue problem for the respective functional Hamiltonian B.

§ 9. Functional Replacement

In this paragraph we establish an explicit expression of the Φ-functional.

Theorem 9.1

The Φ-functional is given by

$$\Phi_{\Psi\chi} = \psi(iu + iv^+)^+ \chi(iv^+)\,\Omega_{uv}\,. \tag{9.1}$$

To prove this we need two lemmata.

Lemma 9.2

The Φ-functional is equal to the element

$$\psi(a^+)^+ V\chi(a^+)\,\Omega \tag{9.2}$$

restricted to $\Omega_a \hat{\otimes} \mathscr{H}_{\Omega_{uv}}$.

Proof: We start from definition (7.6) and determine

$$\begin{aligned}\langle\Phi' \,|\, \Phi_{\Psi\chi}\rangle &:= \langle\Psi \hat{\otimes} \Phi' \,|\, V(\chi \hat{\otimes} \Omega_{uv})\rangle \\ &= \langle\psi(a^+)\,\varphi'(u^+, v^+)\,\Omega \,|\, V\chi(a^+)\,\Omega\rangle \\ &= \langle\Omega_a \hat{\otimes} \Phi' \,|\, \psi(a^+)^+ V\chi(a^+)\,\Omega\rangle\,. \quad \blacksquare\end{aligned}$$

Expression (9.2) still contains operators of the system algebra $\mathfrak{A}_a$. These can be replaced by operators of the functional algebra $\mathfrak{A}_{uv}$ in a well defined manner.

Lemma 9.3. (Replacement of Operator Monoms by Functional Operators)

Let A be an arbitrary element of $\mathfrak{A}_a$ and $M \subseteq \mathscr{N}$. Then

$$a^M VA\,\Omega = (-iu^+ - iv)^M VA\,\Omega\,, \tag{9.3}$$

$$(a^+ + iv^+)^M VA\,\Omega = (-iu + iv^+)^M VA\,\Omega\,. \tag{9.4}$$

Interpretation: If the generating operator is applied to the vacuum state relative to the functional space (Ω_{uv}), then creation/annihilation operators of the system algebra $\mathfrak{A}_a$ preceding the generating operator may be replaced by corresponding linear combinations of operators of the test-algebra.

Proof: Let $\mu \in \mathscr{N}$, then we have

$$\begin{aligned} v_\mu VA\,\Omega &= v_\mu e^{iu^+\cdot a^+} e^{iv^+\cdot a} A\,\Omega \\ &= e^{iu^+\cdot a^+} e^{iv^+\cdot a} e^{-iv^+\cdot a} v_\mu e^{iv^+\cdot a} A\,\Omega \\ &\underset{(\text{I.2.25})}{=} e^{iu^+\cdot a^+} e^{iv^+\cdot a} (v_\mu + ia_\mu) A\,\Omega \\ &= e^{iu^+\cdot a^+} ia_\mu e^{-iu^+\cdot a^+} e^{iu^+\cdot a^+} e^{iv^+\cdot a} A\,\Omega \\ &\underset{(\text{I.2.25})}{=} i(a_\mu + iu_\mu^+)\, VA\,\Omega \end{aligned}$$

from which follows

$$a_\mu VA\,\Omega = (-iv_\mu - iu_\mu^+)\, VA\,\Omega\,. \tag{9.5}$$

By induction we prove (9.3). By an analogue calculation we get

$$u_\mu VA\,\Omega = ia_\mu^+ VA\,\Omega\,,$$

and again (9.4) is deduced by induction. $\blacksquare$

We now prove Theorem 9.1:

A further transformation of (9.2) leads to

$$\begin{aligned} &\psi(a^+)^+ V\chi(a^+)\,\Omega \\ &= \sum_{M \subseteq \mathscr{N}} (-1)^{\frac{1}{2}|M|(|M|-1)}\, \bar{\psi}_M\, a^M V\chi(a^+)\,\Omega \\ &\underset{(9.3)}{=} \sum_{M \subseteq \mathscr{N}} (-1)^{\frac{1}{2}|M|(|M|-1)}\, \bar{\psi}_M (-iu^+ - iv)^M \\ &\quad \cdot V\chi(a^+)\,\Omega \\ &= \psi(iu + iv^+)^+ V\chi(a^+)\, V^{-1} V\Omega \\ &= \psi(iu + iv^+)^+ \chi(a^+ + iv^+)\, V\Omega \\ &\underset{(9.4)}{=} \psi(iu + iv^+)^+ \chi(-iu + iv^+)\, V\Omega\,. \end{aligned} \tag{9.6}$$

With this result the Φ-functional is

$$\begin{aligned} \langle u^{+M} v^{+N}\,\Omega \,|\, \Phi_{\Psi\chi}\rangle &= \langle u^{+M} v^{+N}\,\Omega \,|\, \psi(a^+)^+ V\chi(a^+)\,\Omega\rangle \\ &= \langle u^{+M} v^{+N}\,\Omega \,|\, \psi(iu + iv^+)^+ \chi(-iu + iv^+)\, e^{iu^+\cdot a^+} e^{iv^+\cdot a}\,\Omega\rangle \\ &\underset{(9.6)}{=} \langle u^{+M} v^{+N}\,\Omega \,|\, \psi(iu + iv^+)^+ \chi(-iu + iv^+)\,\Omega\rangle\,. \\ &\underset{(\text{I.2.28})}{} \end{aligned}$$

Comparison of the right-hand factors in the scalar product results in (9.1) according to Riesz' lemma.

Remark: Using the replacement procedures shown in Lemma 9.3 we can immediately give an explicit expression for the functional Hamiltonian

$$B = h^{\triangle}(u^+ + v, u) - h(-iu + iv^+, -iv). \quad (9.7)$$

This way is taken in [8]. We thus have an explicit formulation of functional quantum mechanics without referring to the structural analysis developed in the next paragraph. But the deduction of the functional Hamiltonian (9.7) is greatly simplified by the method of the next paragraph, so we postpone the proof of (9.7).

§ 10. Structural Analysis of the NTD-procedure: Equivalence with a Product of Schrödinger Problems

The explicit expression (9.1) immediately leads to

$$\begin{aligned}\Phi_{\psi\chi} &= \psi(iu + iv^+)^+ \chi(iv^+)\Omega \\ &= e^{-u\cdot v}\psi(iu)^+ e^{u\cdot v}\chi(iv^+)\Omega \\ &= e^{-u\cdot v}\psi(u^+)^{\triangle}\chi(iv^+)\Omega. \end{aligned} \quad (10.1)$$

Following the thesis of Symanzik [15], who introduced a similar transformation in the case of the anharmonic oscillator, we call the operator

$$e^{-u\cdot v} \quad (10.2)$$

the *Symanzik-transformation*. With this transformation, functional quantum mechanics can easily be characterized:

Theorem 10.1. (*Structure of Functional Quantum Mechanics*)

The Symanzik-transformation is a vector space isomorphism from the tensor product $\mathscr{H}_{\Omega_u}(\mathscr{C}) \otimes \mathscr{H}_{\Omega_v}(\mathscr{C})$ *onto the functional space* $\mathscr{F}$. *The* Φ*-functional is given by*

$$\Phi_{\psi\chi} = e^{-u\cdot v}(\psi(u^+)^{\triangle}\chi(iv^+)\Omega), \quad (10.3)$$

the functional Hamiltonian by

$$B = e^{-u\cdot v}(h(u^+, u)^{\triangle} - h(iv^+, -iv))\, e^{u\cdot v} \quad (10.4)$$

or explicitly

$$B = h^{\triangle}(u^+ + v, u) - h(iv^+ - iu, -iv). \quad (10.5)$$

Proof: The Symanzik-transformation is linear, its inverse being $e^{u\cdot v}$; therefore, its an isomorphism of vector spaces. Relation (10.3) was shown at the beginning of the paragraph. Further we have

$$\begin{aligned} B\Phi_{\psi\chi} &:= \Phi_{(H\psi)\chi} - \Phi_{\psi(H\chi)} \\ &\overset{(8.2)}{=} e^{-u\cdot v}((H\psi(u^+)\Omega_u)^{\triangle} \hat{\otimes} \chi(iv^+)\Omega_v \\ &\overset{(10.3)}{=} - \psi(u^+)^{\triangle}\Omega_u \hat{\otimes} h(iv^+, -iv) \\ &\quad \cdot \chi(iv^+)\Omega_v) \\ &= e^{-u\cdot v}(h(u^+, u)^{\triangle} - h(iv^+, -iv) \\ &\quad \cdot \psi(u^+)^{\triangle}\chi(iv^+)\Omega \\ &= e^{-u\cdot v}(h(u^+, u)^{\triangle} - h(iv^+, -iv)) \\ &\quad \cdot e^{u\cdot v}\Phi_{\psi\chi}. \end{aligned}$$

Thus we have (10.4). If we define $H_{iv^+} := h(iv^+, -iv)$, then

$$B = e^{-u\cdot v}(H^{\triangle} \hat{\otimes} I - I \hat{\otimes} H_{iv^+})\, e^{u\cdot v}. \quad (10.6)$$

∎

The Φ-system is given by the Symanzik-transformation of the eigenvalue equation

$$\begin{aligned}&(H^{\triangle} \hat{\otimes} I - I \hat{\otimes} H_{iv^+})(\Psi^{\triangle} \hat{\otimes} \chi_{iv^+}) \\ &= \omega(\Psi^{\triangle} \hat{\otimes} \chi_{iv^+}). \end{aligned} \quad (10.7)$$

This is the tensor product of the conjugate of the Schrödinger problem with the Schrödinger problem itself. From I, Theorem 4.2 we know the conjugate problem being equivalent to the original one. According to [16], I, p. 300, Theorem VIII.33, the spectrum of the tensor product is given by $\sigma_H - \sigma_H$. So we have shown again the equivalence of the Φ-system with the Schrödinger problem.

In the following we denote the difference Hamiltonian by

$$\mathbb{H} := h^{\triangle}(u^+, u) - h(iv^+, iv). \quad (10.8)$$

This operator is selfadjoint. Equation (10.7) therefore can be handled as usual. The Symanzik-transformation provides a relation between the tensor product space, which has a physical interpretation, on one side, and the calculus in the functional space on the other side. This will be evaluated in the next paragraphs.

§ 11. Physical Norm and Physical Inner Product in the Functional Space

We can form the formal inner product with two elements of the functional space $\Phi, \Phi' \in \mathscr{F}$

$$\langle \Phi \,|\, \Phi' \rangle, \quad (11.1)$$

if we consider Φ and Φ' as elements of the Hilbert space $\mathscr{H}_{\Omega_{uv}}(\mathscr{C} \oplus \mathscr{C})$. But this inner product is non-physical. Namely by application of the Symanzik-transformation we get

$$\begin{aligned}\langle \Phi_{\Psi\chi} \,|\, \Phi_{\Psi'\chi'} \rangle = \langle \psi^{\triangle}(u^+ + v)\, \chi(-iv^+ - iu)\Omega \\ \cdot\, |\, \psi'^{\triangle}(u^+ + v) \\ \cdot\, \chi'(iv^+ - iu)\Omega \rangle . \end{aligned} \tag{11.2}$$

If we calculate, e.g., the formal inner product of the one-particle states $\Psi = a_1{}^+\Omega$, $\chi = a_1{}^+\Omega$ and the zero-particle states $\Psi' = \Omega$, $\chi' = \Omega$, we get

$$\langle \Phi_{\Psi\chi} \,|\, \Phi_{\Psi'\chi'} \rangle = -1 ,$$

contrary to the fact, that the transition amplitude from $\Psi^{\triangle} \hat{\otimes} \chi$ to $\Psi'^{\triangle} \hat{\otimes} \chi'$ vanishes.

On the other hand, the inner product on the tensor product space given by the sesquilinear extension of

$$\langle \Psi^{\triangle} \hat{\otimes} \chi \,|\, \Psi'^{\triangle} \hat{\otimes} \chi' \rangle := \langle \Psi^{\triangle} \,|\, \Psi'^{\triangle} \rangle \langle \chi \,|\, \chi' \rangle \tag{11.3}$$

has the physical meaning of the probability amplitude to find the prepared states $\Psi^{\triangle} \otimes \chi$ during a decision measurement for the states $\Psi'^{\triangle} \hat{\otimes} \chi'$. We can transfer this interpretable inner product to the functional space by means of the Symanzik-transformation and the definition:

$$\langle\langle \Phi_{\Psi\chi} \,|\, \Phi_{\Psi'\chi'} \rangle\rangle := \langle \Psi^{\triangle} \hat{\otimes} \chi \,|\, \Psi'^{\triangle} \hat{\otimes} \chi' \rangle . \tag{11.4}$$

We call $\langle\langle .\,|\,. \rangle\rangle$ the physical inner product.

Theorem 11.1

The physical inner product is given by

$$\langle\langle \Phi_{\Psi\chi} \,|\, \Phi_{\Psi'\chi'} \rangle\rangle = \langle \Phi \,|\, G\Phi' \rangle \tag{11.5}$$

with the metric tensor $G := e^{v^+ \cdot u^+} e^{u \cdot v}$. *The functional space is a Hilbert space with* $\langle\langle .\,|\,. \rangle\rangle$ *and the Symanzik-transformation is a unitary mapping of* $(\mathscr{H}_{\Omega}^{\triangle} \hat{\otimes} \mathscr{H}_{\Omega}, \langle .\,|\,. \rangle)$ *onto* $(\mathscr{F}, \langle\langle .\,|\,. \rangle\rangle)$. *Functional quantum mechanics is then unitarily equivalent to the tensor product of the Schrödinger problems.*

Proof:

$$\begin{aligned}&\langle\langle \Phi_{\Psi\chi} \,|\, \Phi_{\Psi'\chi'} \rangle\rangle \\ &= \langle \psi^{\triangle}(u^+)\, \chi(iv^+)\Omega \,|\, \psi'^{\triangle}(u^+)\, \chi'(iv^+)\Omega \rangle \\ &= \langle e^{u \cdot v} \Phi_{\Psi\chi} \,|\, e^{u \cdot v} \Phi_{\Psi'\chi'} \rangle \\ &= \langle \Phi_{\Psi\chi} \,|\, e^{v^+ \cdot u^+} e^{u \cdot v} \Phi_{\Psi'\chi'} \rangle .\end{aligned}$$

Thus $G := e^{u^+ \cdot v^+} e^{u \cdot v}$ is indeed the metric tensor of the physical inner product with respect to the formal inner product. The Symanzik-transformation is a linear mapping from $(\mathscr{H}_{\Omega}^{\triangle} \hat{\otimes} \mathscr{H}_{\Omega}, \langle .\,|\,. \rangle)$ onto $(\mathscr{F}, \langle\langle .\,|\,. \rangle\rangle)$ which preserves inner products and is invertible. Thus $\mathscr{F}$ is indeed a Hilbert space with $\langle\langle .\,|\,. \rangle\rangle$ and $e^{-u \cdot v}$ is unitary. ∎

Theorem 11.1 shows that for convergence examinations in functional space the physical norm

$$|||\, \Phi_{\Psi\chi} \,||| := \sqrt{\langle\langle \Phi_{\Psi\chi} \,|\, \Phi_{\Psi\chi} \rangle\rangle}$$

(or other topologies derived from the physical inner product) must be used to get interpretable results.

§ 12. The Truncated Φ-system

Applying the NTD-procedure, approximate solutions of the eigenvalue problem can be contained by truncating the Φ-system. Instead of solving the Φ-system

$$\begin{aligned}\sum_{K,\, L \subseteq \mathscr{N}} \langle u^{+M} v^{+N} \Omega \,|\, B\, u^{+K} v^{+L} \Omega \rangle\, \varphi(K \,|\, L) \\ = \omega\, \varphi(M \,|\, N)\end{aligned} \tag{12.1}$$

(for all $M, N \subseteq \mathscr{N}$) we are looking for solutions of

$$\begin{aligned}\sum_{\substack{K \in \mathscr{P} \\ L \in \mathscr{P}}} \langle u^{+M} v^{+N} \Omega \,|\, B\, u^{+K} v^{+L} \Omega \rangle\, \varphi(K \,|\, L) \\ = \omega\, \varphi(M \,|\, N)\end{aligned} \tag{12.2}$$

(for all $M, N \in \mathscr{P}$). Here $\mathscr{P} = \{M \subseteq \mathscr{N} \,|\, |M| \leqq p\}$, i.e. in the system (12.1), all powers of creation operators higher than p are put equal to zero. Notice that the expansions (12.1) and (12.2) are made with respect to the formal (i.e. non-physical) inner product. Therefore, we cannot interprete Eq. (12.2) as a p-particle approximation, since the non-orthogonality of the basis $u^{+M} v^{+N}$ with respect to the physical inner product leads to a mixing with higher terms.

Let us define the truncating projection operator P_p by

$$P_p \Phi := \sum_{\substack{M,\, N \subseteq \mathscr{N} \\ |M|,\, |M| \leqq p}} u^{+M} v^{+N} \Omega \langle u^{+M} v^{+N} \Omega \,|\, \Phi \rangle . \tag{12.3}$$

The truncated Φ-system is now the eigenvalue problem

$$P_p B P_p \Phi = \omega_p \Phi \tag{12.4}$$

with the additional condition $P_p \Phi \neq 0$.

Theorem 12.1

Let

$$Q_p := e^{u \cdot v} P_p e^{-u \cdot v} \quad (p \in \mathscr{N}) , \tag{12.5}$$

then Q_p is a non-orthogonal projection operator in the tensor product space. The truncated NTD-procedure is equivalent to the truncated eigenvalue problem

$$Q_p \mathbb{H} Q_p(\Psi^{\triangle} \hat{\otimes} \chi) = \omega_p(\Psi^{\triangle} \hat{\otimes} \chi) \tag{12.6}$$

with the additional condition $Q_p(\Psi^{\triangle} \hat{\otimes} \chi) \neq 0$.

Proof:

$$Q_p{}^2 = e^{u\cdot v} P_p e^{-u\cdot v} e^{u\cdot v} P_p e^{-u\cdot v} = e^{u\cdot v} P_p e^{-u\cdot v},$$

i.e. Q_p is a projection operator.

$$Q_p{}^+ = e^{-v^+\cdot u^+} P_p e^{v^+\cdot u^+} \neq Q_p \quad (p \neq 0)$$

shows that Q_p is non-orthogonal. If we apply the Symanzik-transformation to the truncated Φ-system, we get on the left-hand side

$$\begin{aligned} e^{u\cdot v} P_p B P_p \Phi &= e^{u\cdot v} P_p e^{-u\cdot v} e^{u\cdot v} B e^{-u\cdot v} \\ &\quad \cdot e^{u\cdot v} P_p e^{-u\cdot v} e^{u\cdot v} \Phi \\ &= Q_p \mathbb{H} Q_p e^{u\cdot v} \Phi, \end{aligned}$$

thus

$$Q_p \mathbb{H} Q_p e^{u\cdot v}\Phi = \omega_p e^{u\cdot v}\Phi$$

with the condition $Q_p e^{u\cdot v}\Phi \neq 0$. ∎

In the following we collect some properties of the truncating projection operators Q_p. A detailed analysis of these operators is a prerequisite for the treatment of convergence in the NTD-procedure.

Theorem 12.2

The truncating projection operators Q_p can be split up into

$$Q_p = P_p + R_p \tag{12.7}$$

there P_p is the orthogonal projector onto the subspace with particle number $\leqq p$ and R_p is given by

$$R_p = -P_p \sum_{|Q|>p} \left(\sum_{r>p} \binom{|Q|}{|Q|-r} (-1)^r \right) (u\,v)^Q . \tag{12.8}$$

The following identities hold:

$$\begin{aligned} &P_p Q_p = Q_p, \quad P_p R_p = R_p, \\ &R_p P_p = 0. \end{aligned} \tag{12.9}$$

Proof: Let $\Phi \in \mathcal{F}$ be arbitrary. Then

$$\begin{aligned} Q_p\Phi &= e^{u\cdot v} P_p e^{-u\cdot v}\Phi = e^{u\cdot v} \sum_{|K|,\,|L|\leq p} u^{+K} v^{+L} \Omega \langle u^{+K} v^{+L} \Omega \,|\, e^{-u\cdot v}\Phi\rangle \\ &= \sum_{|K|,\,|L|\leq p} (u^+ - v)^K v^{+L} \Omega \langle u^{+K} v^{+L} \Omega \,|\, e^{-u\cdot v}\Phi\rangle \\ &= \sum_{|K|,\,|L|\leq p} \sum_{R\subseteq K\cap L} (-1)^{\frac{1}{2}|R|(|R|-1)} \operatorname{sign}(K\setminus R \,|\, R) \operatorname{sign}(R \,|\, L\setminus R)\, u^{+K\setminus R} (-1)^{|R|} v^{+L\setminus R}\Omega \\ &\quad \cdot \langle \operatorname{sign}(K\setminus R \,|\, R) \operatorname{sign}(R \,|\, L\setminus R)\, u^{+K\setminus R} u^{+R} v^{+R} v^{+L\setminus R}\Omega \,|\, e^{-u\cdot v}\Phi\rangle . \end{aligned}$$

Now

$$\begin{aligned} &\langle u^{+K\setminus R} u^{+R} v^{+R} v^{+L\setminus R}\Omega \,|\, e^{-u\cdot v}\Phi\rangle = \langle u^{+R} v^{+R} u^{+K\setminus R} v^{+L\setminus R}\Omega \,|\, e^{-u\cdot v}\Phi\rangle \\ &= \langle u^{+K\setminus R} v^{+L\setminus R}\Omega \,|\, v^R u^R e^{-u\cdot v}\Phi\rangle = \langle u^{+K\setminus R} v^{+L\setminus R}\Omega \,|\, (-1)^{\frac{1}{2}|R|(|R|+1)} (u\,v)^R e^{-u\cdot v}\Phi\rangle . \end{aligned}$$

In the last expression we collect all terms with $u^{+M} v^{+N}\Omega$ for constant $M, N \subseteq \mathcal{N}$. This term occurs as many times as $M \cup R = K$ with $|K| \leqq p$ and $N \cup R = L$ with $|L| \leqq p$ is valid for R with $M \cap R = N \cap R = \emptyset$. Thus

$$\begin{aligned} Q_p\Phi &= \sum_{M,\,N\subseteq\mathcal{N}} \sum_{\substack{R\subseteq\mathcal{N}\setminus(M\cup N) \\ |M\cup R|\leq p \\ |N\cup R|\leq p}} u^{+M} v^{+N}\Omega \langle u^{+M} v^{+N}\Omega \,|\, (u\,v)^R e^{-u\cdot v}\Phi\rangle \\ &= \sum_{|M|,\,|N|\leq p} u^{+M} v^{+N}\Omega \left\langle u^{+M} v^{+N}\Omega \,\middle|\, \left(\sum_{R\subseteq\mathcal{N}} (u\,v)^R - \sum_{|R|>p} (u\,v)^R \right) e^{-u\cdot v}\Phi \right\rangle \\ &= P_p \left(\sum_{R\subseteq\mathcal{N}} (u\,v)^R e^{-u\cdot v} - \sum_{|R|>p} (u\,v)^R e^{-u\cdot v} \right) \Phi \\ &= \left(P_p - P_p \sum_{\substack{|R|>p \\ S\subseteq\mathcal{N}}} (u\,v)^R (-u\,v)^S \right) \Phi \\ &= \left(P_p - P_p \sum_{|Q|>p} \left(\sum_{r>p} \binom{|Q|}{|Q|-r} (-1)^r \right) (u\,v)^Q \right) \Phi \end{aligned} \tag{12.10}$$

This proves the assertion (12.7)—(12.8). Equations (12.9) follow immediately from (12.10). ∎

As was shown by the first author [8], for $p=1, 2$ and 4 the truncated system of an exciton model gives results comparable to those obtained by Haken [17]. Theorem 12.2 explains this correspondence: the truncating projection operator Q_p is equal to the projector of the subspace with particle number $\leqq p$ except for the "perturbation" R_p.

The vality of the approximation of $\mathbb{H}$ by

$$Q_p \mathbb{H} Q_p = P_p \mathbb{H} P_p + (P_p \mathbb{H} R_p + R_p \mathbb{H} P_p + R_p \mathbb{H} R_p) \tag{12.11}$$

is given by an estimate of the remaining $R_p \Phi$. However, it can be shown that for certain states Φ the norm of $R_p \Phi$ may be fairly large. In the thermodynamic limit R_p is an unbounded operator.

In this situation we only can try to estimate $R_p \Phi$ at least for the eigenstates of $\mathbb{H}$. Under very restricting conditions on $\mathbb{H}$, Müller [18] could prove the convergence of the NTD-procedure.

The problems of this approximation are caused by the use of non-orthogonal truncating projection operators. In another paper we will give a functional formulation which avoids these difficulties.

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