On the Field Theoretic Functional Calculus for the Anharmonic Oscillator I

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In sections 1, 2, 3, 4 the many-time and one-time functional calculus is developed for the anharmonic oscilator in analogy to the requirements of nonlinear spinor theory. In section 5 the N.T.D.-method is discussed for the eigenvalue functional equation. It is shown that the N.T.D.-method admits different representations, namely a symmetric one and an unsymmetric one. The proof of convergence is given for the symmetric one in section 6. In section 7 the connection between the unsymmetric and the symmetric representation is discussed and in section 8 follow numerical values in comparison with SCHRÖDINGER theory.

In modern quantum theory the dynamical behavior of physical systems (particles, fields) can be described by functionals of field operators in a HEISENBERG representation and corresponding functional equations [1]. In configuration space the functional equations lead to infinite sets of differential or integral equations between the different time ordered matrix elements of the field operators [2]. This description is of special interest, because it is formally valid for canonical as well as for noncanonical quantisation, where the usual SCHRÖDINGER representation is inapplicable [3]. However, up to now no systematic method of solution for these field theoretic functional equations for strong coupling has been given. In nonlinear spinor theory of elementary particles with noncanonical relativistic HEISENBERG quantisation [4], HEISENBERG proposed the socalled New-TAMM–DANCOFF-method (N.T.D.-method) introduced by DYSON [5] as an appropriate approximation scheme for the solution of the functional equations. The transition from canonical to noncanonical quantisation does not change the structure of the corresponding functional equations [6]. Therefore for testing and investigating HEISENBERG's proposal, one should at first consider those theories already regularized by canonical quantisation and compare the results obtained by functional calculus with those obtained from SCHRÖDINGER theory. The simplest example is offered by the anharmonic oscillator, the functional equations of which are analogous to those of nonlinear spinor theory, as is shown in the following. The investigation of this model has been already developed in some papers. At first HEISENBERG calculated the lowest approximations of the one-time-N.T.D.-method in the $p-q$-representation [7], later STUMPF, WAGNER and WAHL [2] and WAGNER [9] proved the convergence of the one-time N.T.D.-method in the q-representation. So one has a first hint of the validity of the method. But of more interest for field theory is the rigorous treatment of the $p-q$-representation, being undertaken in this paper. For this investigation a representation of the generating one-time $p-q$-function, given by SYMANZIK [10] is very useful.

But we do not confine ourselves to a purely theoretical discussion of the subject. In the last section we treat the problem numerically, especially in connection with the question of good numerical convergence raised by the paper of SCHWARTZ [11] in order to get complete information about the theoretical and numerical properties of the N.T.D.-procedure.

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1. Many-Time Functional Representation

The equations of motion for the anharmonic oscillator are

$$\frac{\mathrm{d}}{\mathrm{d}t}\, q(t) = p(t), \qquad \frac{\mathrm{d}}{\mathrm{d}t}\, p(t) = -q^3(t) \tag{1.1}$$

with the commutation relation

$$[p(t), q(t)]_- = -i\mathbf{1}. \tag{1.2}$$

i. e. canonical quantisation. For the solution of this problem we do not use SCHRÖDINGER theory. As mentioned in the introduction we consider the quantized anharmonic oscillator as a simple model for the functional calculus of quantum field theory and study its functional equations. But there are different possibilities for this treatment, namely the q-representation, and the $p-q$-representation. The first is analogous to nonlinear scalar field theory, see ref. [3], the second to nonlinear spinor theory of elementary particles. However, the $p-q$-representation allows the transition to the one-time limit. For this reason we use the $p-q$-representation and give firstly in this and the next sections those relations which are exactly valid.

To give a more concise description, showing at the same time the complete analogy to nonlinear spinor theory, we define the "field operators" $\psi_i(t)$ by $\psi_1(t) := q(t)$ and $\psi_2(t) := p(t)$ and obtain from (1.1) the "field" equation, being analogous to DÜRR and WAGNER's spinor field representation [1]

$$\frac{\mathrm{d}}{\mathrm{d}t}\, \psi_\alpha(t) = B_{\alpha\beta}\, \psi_\beta(t) + C_{\alpha\beta}\, \psi_\beta(t)\; \psi_\gamma(t)\; D_{\gamma\delta}(t)\; \psi_\delta(t) \tag{1.3}$$

and from (1.2) the commutation relation

$$[\psi_\alpha(t), \psi_\beta(t)]_- = \mathbf{1}\, A_{\alpha\beta} \tag{1.4}$$

with

$$A := \begin{pmatrix} 0 & i \\ -i & 0 \end{pmatrix}; \quad B := \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}; \quad C := \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}; \quad D := \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}. \tag{1.5}$$

As is well known the dynamical behavior of the system (1.1) and (1.2) resp. (1.3) and (1.4) can be described by the set of time ordered matrix elements

$$\tau_{nm}^{ab}(t_1 \dots t_n, t_1' \dots t_m') := \langle a \,|\, T\, \psi_1(t_1) \dots \psi_1(t_n)\; \psi_2(t_1') \dots \psi_2(t_m') \,|\, b \rangle \quad (n, m = 0 \dots \infty) \tag{1.6}$$

where $\langle a|$ and $|b\rangle$ are fixed eigenstates of the anharmonic oscillator. Introducing a functional formulation the complete set (1.6) can be obtained from the functional

$$\mathfrak{T}_{ab}(j_1\, j_2) := \langle a \,|\, T \exp\{i \textstyle\int j_\alpha(\xi)\; \psi_\alpha(\xi)\; \mathrm{d}\xi\} |\, b \rangle \tag{1.7}$$

where the right side of (1.7) is an abbreviation of the power series definition

$$\mathfrak{T}_{ab}(j_1\, j_2) := \sum_{nm} \frac{i^{n+m}}{n!\, m!} \int \tau_{nm}^{ab}(t_1 \dots t_n, t_1' \dots t_m') \times j_1(t_1) \dots j_1(t_n)\; j_2(t_1') \dots j_2(t_m')\; \mathrm{d}t_1 \dots \mathrm{d}t_m'. \tag{1.8}$$

Then the equations of motion (1.3) (1.4) can be replaced by a functional equation for $\mathfrak{T}_{ab}(j_1\, j_2)$. This functional equation reads

$$\frac{\mathrm{d}}{\mathrm{d}t}\, \frac{\delta \mathfrak{T}_{ab}}{\delta j_\alpha(t)} = O_\alpha\left(j_1\, j_2, \frac{\delta}{\delta j_1}\, \frac{\delta}{\delta j_2}\right) \mathfrak{T}_{ab} \tag{1.9}$$

with

$$O_\alpha := \left[-A_{\alpha\beta}\, j_\beta(t) + B_{\alpha\beta}\, \frac{\delta}{\delta j_\beta(t)} + C_{\alpha\beta}\, \frac{\delta}{\delta j_\beta(t)}\, \frac{\delta}{\delta j_\gamma(t)}\, D_{\gamma\delta}\, \frac{\delta}{\delta j_\delta(t)} \right]. \tag{1.10}$$

For the rules of functional calculus to deduce equation (1.9) from (1.3) and (1.4) see ref. [3, 12]. The equations for the τ-functions corresponding to (1.9) contain singular parts (δ-functions) connected with the term $A_{\alpha\beta}\, j_\beta(t)$. So the first step on the way to a solution of (1.8) has to be the compensation of these singularities. This can be done according to DYSON [5] by using the WICK-rule as a transformation rule, i. e. by changing the time ordered products into normal ordered products. This normal ordering can be defined independent of the existence of creation and annihilation operators as a functional transformation. This transformation reads

$$\mathfrak{T}_{ab}(j_1\, j_2) = \Phi_{ab}(j_1\, j_2) \times \exp\{-\tfrac{1}{2} \textstyle\int j_\alpha(\xi)\; F_{\alpha\beta}(\xi - \eta)\; j_\beta(\eta)\; \mathrm{d}\xi\, \mathrm{d}\eta\} \tag{1.11}$$

with

$$F_{\alpha\beta}(\xi - \eta) := \langle 0 \,|\, T\, \psi_\alpha(\xi)\; \psi_\beta(\eta) \,|\, 0 \rangle \tag{1.12}$$

and

$$\Phi_{ab}(j_1\, j_2) := \sum_{nm} \frac{i^{n+m}}{n!\, m!}\, \varphi_{nm}^{ab}(t_1 \dots t_n, t_1' \dots t_m') \times j_1(t_1) \dots j_1(t_n)\; j_2(t_1') \dots j_2(t_m')\; \mathrm{d}t_1 \dots \mathrm{d}t_m'. \tag{1.13}$$

The transformed equation (1.9) then reads

$$\frac{\mathrm{d}}{\mathrm{d}t}\, \frac{\mathrm{d}\Phi_{ab}}{\mathrm{d}j_\alpha(t)} = O_\alpha\left(j_1\, j_2, \frac{\mathrm{d}}{\mathrm{d}j_1}\, \frac{\mathrm{d}}{\mathrm{d}j_2}\right) \Phi_{ab} \tag{1.14}$$

[12] K. SYMANZIK, Z. Naturforschg. 10 a, 809 [1954].

if one defines the d-derivation on j_a by

$$\frac{\mathrm{d}}{\mathrm{d}j_a(t)} := \frac{\delta}{\delta j_a(t)} - \int F_{a\beta}(t-\eta)\, j_\beta(\eta)\, \mathrm{d}\eta\,. \qquad (1.15)$$

A more detailed analysis shows that (1.14) in configuration space of φ-function is a system of equations completely free of singular expressions, because the functions (1.12) are regular functions for the anharmonic oscillator with canonical quantisation. For field theories however the analogous functions to (1.12) are still singular. (1.9) resp. (1.14) does not contain all the information about the functions $\mathfrak{T}_{ab}$ resp. Φ_{ab} that can be obtained from the theory. In the next section we show that there are still other relations, which have to be fulfilled in order to get the exact physical functionals.

2. Necessary Subsidiary Conditions

For any matrix element of field operators we have, according to the translational covariance of the theory, necessary subsidiary conditions, when the projection states are eigenstates of energy and momentum, see ref. [2]. For the anharmonic oscillator these conditions are reduced to one condition for time translational invariance. We formulate this condition in functional description. It reads for the $\mathfrak{T}$-functional

$$\int j_a(t)\, \frac{\mathrm{d}}{\mathrm{d}t}\, \frac{\delta}{\delta j_a(t)}\, \mathrm{d}t\; \mathfrak{T}_{ab}(j_1\, j_2) = i\, \omega_{ab}\, \mathfrak{T}_{ab}(j_1\, j_2) \quad (2.1)$$

with $\omega_{ab} := (E_a - E_b)$ and because the Φ-functional is constructed from field operators too, the same relation holds for this functional. So we have

$$\int j_a(t)\, \frac{\mathrm{d}}{\mathrm{d}t}\, \frac{\delta}{\delta j_a(t)}\, \mathrm{d}t\; \Phi_{ab}(j_1\, j_2) = i\, \omega_{ab}\, \Phi_{ab}(j_1\, j_2)\,. \quad (2.2)$$

Now from (1.9) follows by multiplication with $j_a(t)$, integration over t, and comparison with (2.1)

$$i\, \omega_{ab}\, \mathfrak{T}_{ab}(j_1\, j_2) = \int j_a(t)\, O_a\!\left(j_1\, j_2\, \frac{\delta}{\delta j_1}\, \frac{\delta}{\delta j_2}\right) \mathrm{d}t \times \mathfrak{T}_{ab}(j_1\, j_2)\,. \quad (2.3)$$

To derive a similar equation for the Φ-functional, one observes the equality [10]

$$\int j_a(t)\, \frac{\mathrm{d}}{\mathrm{d}t}\, \frac{\mathrm{d}}{\mathrm{d}j_a(t)}\, \mathrm{d}t\; \Phi_{ab}(j_1\, j_2) = \int j_a(t)\, \frac{\mathrm{d}}{\mathrm{d}t}\, \frac{\delta}{\mathrm{d}j_a(t)}\, \mathrm{d}t \times \Phi_{ab}(j_1\, j_2) \quad (2.4)$$

and therefore obtains from (1.14) and (2.2)

$$i\, \omega_{ab}\, \Phi_{ab}(j_1\, j_2) = \int j_a(t)\, O_a\!\left(j_1\, j_2\,, \frac{\mathrm{d}}{\mathrm{d}j_1}\, \frac{\mathrm{d}}{\mathrm{d}j_2}\right) \mathrm{d}t \times \Phi_{ab}(j_1\, j_2)\,. \quad (2.5)$$

(2.3) resp. (2.5) is the functional substitute for the Hamiltonian. It is a subsidiary condition which is automatically satisfied, if the equations (1.9) and (2.1) resp. (1.14) and (2.2) are satisfied. But it is not sufficient for the calculation of the functionals $\mathfrak{T}_{ab}$ resp. Φ_{ab} themselves. So one cannot replace for actual calculations of $\mathfrak{T}_{ab}$ resp. Φ_{ab} the equations (1.9) and (2.1) resp. (1.14) and (2.2) by (2.3) resp. (2.5). Nevertheless from their character as necessary subsidiary conditions (2.3) and (2.5) are useful for the calculation of eigenvalues. Because no time derivation appears in (2.5) this equation can still be simplified by the transition to the one-time formalism. In the configuration space of τ- resp. φ-functions this transition means, to put all times $t_1 \ldots t_n$, $t_1' \ldots t_m'$ equal to zero. But one has to be cautious, because the τ-functions are discontinuous functions for equal times. So their values depend on the way the limiting process is performed. But there exists a well defined limiting procedure leading exactly to the usual one-time symmetrized τ-functions. Defining them by

$$\tau_{nm}^{ab}(0\,|\,0) := \langle a\,|\,\mathrm{Sym}\, q^n(0)\; p^m(0)\,|\,b\rangle \qquad (2.6)$$

we then get (2.6) by the following operation from (1.6)

$$\tau_{nm}^{ab}(0\,|\,0) \equiv \overset{n\;m}{\mathrm{Lim}}\; \tau_{nm}^{ab}(t_1 \ldots t_n, t_1' \ldots t_m') \qquad (2.7)$$

where the operator Lim is defined by

$$\overset{nm}{\mathrm{Lim}}\; \tau_{nm}^{ab}(t_1 \ldots t_n, t_{n+1} \ldots t_{m+n}) := \int L(t_1 \ldots t_{m+n})\, \tau_{nm}^{ab}(t_1 \ldots t_{m+n})\, \mathrm{d}t_1 \ldots \mathrm{d}t_{m+n} \qquad (2.8)$$

with

$$L(t_1 \ldots t_{m+n}) := \frac{1}{(m+n)\,!} \sum_{\mathrm{Per.}\, \varepsilon_{i_1} > \ldots > \varepsilon_{i_{m+n}}} \lim_{\varepsilon_i \to 0} \delta(t_1 - \varepsilon_{i_1}) \ldots \delta(t_{m+n} - \varepsilon_{i_{m+n}})\,. \qquad (2.9)$$

Therefore the transition to the one-time formalism can be directly performed in functionals by substituting

$$j_1(t_1) \ldots j_1(t_n)\; j_2(t_{n+1}) \ldots j_2(t_{m+n})\; \mathrm{d}t_1 \ldots \mathrm{d}t_{m+n} = L(t_1 \ldots t_{m+n})\; x^n\, y^m\; \mathrm{d}t_1 \ldots \mathrm{d}t_{m+n} \qquad (2.10)$$

with $j_1(0) =: x$ and $j_2(0) =: y$. Then we denote the one-time limit for the $\mathfrak{T}$-functional as

$$\mathrm{Lim}\, \mathfrak{T}_{ab}(j_1\, j_2) := \frac{i^{n+m}}{n\,!\; m\,!} \sum_{n,m} \int \tau_{nm}^{ab}(t_1 \ldots t_{m+n}) \times L(t_1 \ldots t_{m+n})\, x^n\, y^m\, \mathrm{d}t_1 \ldots \mathrm{d}t_{m+n} = \sum_{n,m} \frac{i^{n+m}}{n\,!\; m\,!}\, \tau_{ab}(n\,|\,m)\; x^n\, y^m =: T_{ab}(x, y) \quad (2.11)$$

with

$$\tau_{ab}(n \mid m) := \tau^{ab}_{nm}(0 \mid 0). \quad (2.12)$$

In contrast to the τ-functions the φ-functions are continuous functions in their time variables. So for these functions one can put all times to zero without any complication. But one could apply the Lim operator (2.9) on the Φ-functional too, obtaining

$$\text{Lim}\ \Phi_{ab}(j_1 j_2) = \sum_{n,m} \frac{i^{n+m}}{n!\,m!} \varphi_{ab}(n \mid m)\, x^n\, y^m =: \Phi_{ab}(x, y) \quad (2.13)$$

with

$$\varphi_{ab}(n \mid m) := \varphi^{ab}_{nm}(0 \mid 0) := \lim \varphi^{ab}_{nm}(t_1 \dots t_n, t_1' \dots t_m'). \quad (2.14)$$

Of course, both methods give the same results in this case.

Having performed the limiting procedure for the functionals, one would like to do the same for the corresponding functional equations. Taking firstly equation (2.3) one observes, that it is impossible to apply the Lim operator to it, because in configuration space (2.3) gives equations containing already τ-functions of equal arguments in the many-time description. So the operator Lim is inapplicable to (2.3). This difficulty does not arise in the equation (2.5) for the Φ-functional, because the φ-functions are continuous functions. Only the operator O_α contains discontinuous parts. The transition to the one-time limit can the be performed by the application of the relation

$$\text{Lim}[\mathfrak{f}(j_1 j_2)\ \Phi_{ab}(j_1 j_2)] = \text{Lim}\ \mathfrak{f}(j_1 j_2)\ \text{Lim}\ \Phi_{ab}(j_1 j_2) \quad (2.15)$$

where $\mathfrak{f}(j_1 j_2)$ is an arbitrary functional, whose expansion functions $f_r(t_1 \dots t_r)$ may be discontinuous functions in the time variables. Replacing further all free $j(t)$ which are not integrated by $j(0)$, one may apply the Lim-operator on (2.5), obtaining by use of (2.15)

$$i\,\omega_{ab}\,\Phi_{ab}(x, y) = \left[\text{Lim} \int j_\alpha(t)\ O_\alpha\left(j_1 j_2, \frac{\mathrm{d}}{\mathrm{d}j_1} \frac{\mathrm{d}}{\mathrm{d}j_2}\right) \mathrm{d}t\right] \Phi_{ab}(x, y). \quad (2.16)$$

In appendix I it is shown that the Lim procedure on O_α leads to

$$\text{Lim} \int j_\alpha(t)\ O_\alpha\left(j_1 j_2, \frac{\mathrm{d}}{\mathrm{d}j_1} \frac{\mathrm{d}}{\mathrm{d}j_2}\right) \mathrm{d}t =: \mathfrak{W}\left(x, y, \frac{\mathrm{d}}{\mathrm{d}x} \frac{\mathrm{d}}{\mathrm{d}y}\right) \quad (2.17)$$

with

$$\frac{\mathrm{d}}{\mathrm{d}x} := \frac{\partial}{\partial x} - F_{11}(0)\, x; \quad \frac{\mathrm{d}}{\mathrm{d}y} := \frac{\partial}{\partial y} - F_{22}(0)\, y \quad (2.18)$$

and

$$\mathfrak{W}\left(x, y, \frac{\partial}{\partial x} \frac{\partial}{\partial y}\right) := x \frac{\partial}{\partial y} - \tfrac{1}{4} y^3 \frac{\partial}{\partial x} + y \frac{\partial^3}{\partial x^3}. \quad (2.19)$$

So one has the equation

$$i\,\omega_{ab}\,\Phi_{ab}(x, y) = \mathfrak{W}\left(x, y, \frac{\mathrm{d}}{\mathrm{d}x} \frac{\mathrm{d}}{\mathrm{d}y}\right) \Phi_{ab}(x, y) \quad (2.20)$$

for the Φ-functional in the one-time limit. Applying the Lim-operator (2.8) to (1.11) one obtains by the rule (2.15)

$$\begin{aligned} T_{ab}(x, y) &= \Phi_{ab}(x, y)\ \text{Lim} \exp - \tfrac{1}{2} \int j_\alpha(\xi)\, F_{\alpha\beta}(\xi - \eta)\, j_\beta(\eta)\, \mathrm{d}\xi\, \mathrm{d}\eta \\ &= \Phi_{ab}(x, y) \exp\left(-\frac{\Delta}{2} x^2 - \frac{\Gamma}{2} y^2\right) \end{aligned} \quad (2.21)$$

with $\Delta := F_{11}(0)$ and $\Gamma := F_{22}(0)$. This gives with (2.18), (2.19) and (2.20) the equation

$$i\,\omega_{ab}\,T_{ab}(x, y) = \mathfrak{W}\left(x, y, \frac{\partial}{\partial x} \frac{\partial}{\partial y}\right) T_{ab}(x, y). \quad (2.22)$$

In principle this equation is sufficient to construct the many-time functionals too, if one is able to calculate all eigenvalues ω_{ab}.

3. One-Time Functional Representation

Independent from our deductions in the preceding sections we now consider the one-time functional representation, using the HAMILTONIAN of (1.1) for the derivation of the functional equation. Finally we shall connect the results obtained here, with those of the preceding sections. To begin with, we define the generating one-time function by

$$T_{ab}(x, y) := \langle a \mid \exp(i\,x\,q + i\,y\,p) \mid b \rangle \quad (3.1)$$

being an abbreviated expression for the power series expansion

$$T_{ab}(x, y) := \sum_{n,m} \frac{i^{n+m}}{n!\,m!} \tau_{ab}(n \mid m)\, x^n\, y^m \quad (3.2)$$

where the expansion coefficients are defined by (2.6) and (2.12). The time dependence of (3.1) can be evaluated by using the formula $i\,R = [H, R]_-$ valid for any operator R of p and q and identifying R with $\exp(i\,x\,q + i\,y\,p)$. Then one gets by multiplying this equation from the left with $\langle a \mid$ and from the right with $\mid b \rangle$ the equation for T_{ab}

$$\omega_{ab}\,T_{ab}(x, y) = W\left(x, y, \frac{\partial}{\partial x} \frac{\partial}{\partial y}\right) T_{ab}(x, y) \quad (3.3)$$

with

$$W\left(x, y, \frac{\partial}{\partial x}\frac{\partial}{\partial y}\right) := x\frac{1}{i}\frac{\partial}{\partial y} - \frac{1}{4}y^3\frac{1}{i}\frac{\partial}{\partial x} - y\left(\frac{1}{i}\frac{\partial}{\partial x}\right)^3. \quad (3.4)$$

In the HILBERT space $\mathfrak{L}^2$ of square integrable functions $f(x, y)$ of two variables x and y with domain S, where S is the space of infinitly often differentiable rapidly decreasing functions, W is an essentially selfadjoint operator. Its spectrum can easily be gained by a unitary transformation in $\mathfrak{L}^2$ Putting according to SYMANZIK [10]

$$T(x, y) = (U\,\Psi)(x, y) := \int \exp(i\,x\,\xi)\,\Psi\left(\xi - \frac{y}{2}, \xi + \frac{y}{2}\right)\mathrm{d}\xi \quad (3.5)$$

and

$$\Psi(\xi, \eta) = (U^{-1}T)(\xi, \eta) := (2\pi)^{-1}\int \exp\{-i\frac{x}{2}(\xi+\eta)\}\times T(x, \xi-\eta)\,\mathrm{d}x \quad (3.6)$$

from (3.3) and (3.4) follows, that Ψ fulfills the equation

$$\omega\,\Psi = U^{-1}\,W\,U\,\Psi \quad (3.7)$$

having the same eigenvalue spectrum as (3.2). Explicitly the transformed operator is given by

$$U^{-1}\,W\,U := H(\xi) - H(\eta) \quad (3.8)$$

where H is the HAMILTONIAN of the anharmonic oscillator.

$$H(x) := -\frac{1}{2}\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \tfrac{1}{4}x^4. \quad (3.9)$$

Therefore the solutions of (3.7) are of the form

$$\Psi_{ab}(\xi, \eta) = \psi_a(\xi)\,\psi_b(\eta) \quad (3.10)$$

where ψ_a and ψ_b are both solutions of

$$H\,\psi = E\,\psi \quad (3.11)$$

with eigenvalues E_a resp. E_b, and so the spectrum of W consists of all $\omega_{ab} = (E_a - E_b)$ where E_a and E_b varies among all eigenvalues of (3.11). Because of (3.5) and (3.10) T_{ab} has to be a square integrable function with

$$\frac{1}{2\pi}\int |T_{ab}(x, y)|^2\,\mathrm{d}x\,\mathrm{d}y = \langle\psi_a\,|\,\psi_a\rangle\,\langle\psi_b\,|\,\psi_b\rangle = 1. \quad (3.12)$$

This condition serves as a boundary condition for the eigensolutions of the operator W. We may expand T_{ab} into the series

$$T_{ab}(x, y) = \Phi_{ab}(x, y)\exp\left(-\frac{\Delta}{2}x^2 - \frac{\Gamma}{2}y^2\right) \quad (3.13)$$

with

$$\Phi_{ab}(x, y) := \sum_{n,m}\frac{i^{n+m}}{n!\,m!}\varphi_{ab}(n\,|\,m)\,x^n\,y^m. \quad (3.14)$$

Identifying Δ with $F_{11}(0)$ and Γ with $F_{22}(0)$ this expansion is identical with the application of the WICK rule on $T_{ab}(x, y)$, see ref. [10]. Inserting (3.13) into (3.3), we obtain the transformed equation

$$\omega_{ab}\,\Phi_{ab}(x, y) = W\left(x, y, \frac{\mathrm{d}}{\mathrm{d}x}\frac{\mathrm{d}}{\mathrm{d}y}\right)\Phi_{ab}(x, y) \quad (3.15)$$

with

$$\frac{\mathrm{d}}{\mathrm{d}x} := \frac{\partial}{\partial x} - \Delta x; \qquad \frac{\mathrm{d}}{\mathrm{d}y} := \frac{\partial}{\partial y} - \Gamma\,y. \quad (3.16)$$

Now we connect the results obtained in this section, with those of section 2. It is easily seen, that we have

$$i\,W\left(x, y, \frac{\partial}{\partial x}\frac{\partial}{\partial y}\right) \equiv \mathfrak{W}\left(x, y, \frac{\partial}{\partial x}\frac{\partial}{\partial y}\right) \quad (3.17)$$

and equations (3.15) and (2.20) are equal. Therefore the many-time formalism without use of the HAMILTONian gives in the one-time limit the same results as the genuine one-time formalism using the HAMILTONian. So the results of this section obtained from HAMILTONian formalism are also valid for the HAMILTONfree many-time formalism in the limit of equal times. Therefore we consider the application of the HAMILTONian in this section only as a labour saving device, but not as a fundamental requirement of the whole theory.

4. Matrix Representations

In the preceding section we have seen, that we may forget about the origin of our "functional operator" W, because its square integrable eigenfunction are just the physical ones. So the problem is, to find approximate eigensolutions or at least eigenvalues of W. To use perturbation theory is clearly unreasonable. Another way is to find a suitable matrix representation of W, which can be truncated; so one gets a finite dimensional eigenvalue problem, which can be solved. In order to do this, we first study two obvious matrix representations.

The first possibility is, to use the WICK rule (3.13) (3.14) for an expansion of $T_{ab}(x, y)$ writing

$$T_{ab}(x, y) = \sum_{n,m=0}^{\infty}\varphi_{ab}(n\,|\,m)\,\langle x\,y\,|\,f_{nm}\rangle \quad (4.1)$$

with

$$\langle x\,y \mid f_{nm}\rangle := \frac{i^{m+n}}{n!\,m!} x^n\, y^m \exp\left(-\frac{\Delta}{2}x^2 - \frac{\Gamma}{2}y^2\right) \quad (4.2)$$

and then find a matrix $W_{hj,\,nm}$ with the property

$$W \mid f_{nm}\rangle = \sum_{h,j} W_{hj,\,nm} \mid f_{hj}\rangle\,. \quad (4.3)$$

The usual field theoretic way to obtain the matrix $W_{hj,\,nm}$ is to compare coefficients of equal powers of x and y on both sides of the eigenvalue equation (3.3) after inserting (4.1). Then the eigenvalue equation reads

$$\sum_{n,m=0}^{\infty} (W_{hj,\,nm} - \omega_{ab}\,\delta_{hn}\,\delta_{jm})\,\varphi_{ab}(n \mid m) = 0\,. \quad (4.4)$$

The explicit form of $W_{hj,\,nm}$ is given in appendix II. But this equations can be gained by the conventional quantum mechanical methods too.

If we define the reziprocal basis $\langle h_{nm} \mid$ by

$$\langle h_{nm} \mid f_{rs}\rangle = \delta_{nr}\,\delta_{ms} \quad (4.5)$$

then we have simply

$$W_{hj,\,nm} := \langle h_{hj}\, W\, f_{nm}\rangle\,. \quad (4.6)$$

Unfortunately the system (4.2) is a complete one, but it forms no basis, i. e. the reciprocal system $\langle h_{nm} \mid$ does not exist in $\mathfrak{L}^2$. It may be formally introduced as a set of linear functionals, which are not continuous on $\mathfrak{L}^2$. This property is very inconvenient for a proof of convergence of our suggested approximation method. As a consequence we look for an orthogonal basis, which clearly does not have this troublesome property, because it is identical with its reciprocal basis. The easiest way to obtain such a basis is to orthonormalize the $\mid f_{nm}\rangle$ of (4.2); so we end up with the orthogonal system of harmonic oscillator functions $\mid \Phi_{nm}\rangle$ defined in appendix II. We then have for T_{ab} the expansion

$$T_{ab}(x,y) = \sum_{n,m=0}^{\infty} \chi_{ab}(n \mid m)\,\langle x\,y \mid \Phi_{nm}\rangle \quad (4.7)$$

and derive from (3.3) by inserting (4.7) and projecting on $\langle \Phi_{hj} \mid$ the set of equations

$$\sum_{n,m=0}^{\infty} (H_{hj,\,nm} - \omega_{ab}\,\delta_{hn}\,\delta_{jm})\,\chi_{ab}(n \mid m) = 0 \quad (4.8)$$

with $$\langle \Phi_{hj} \mid \Phi_{nm}\rangle = \delta_{hn}\,\delta_{jm} \quad (4.9)$$

and $$H_{hj,\,nm} := \langle \Phi_{hj}\, W\, \Phi_{nm}\rangle \quad (4.10)$$

explicitly given in appendix II.

Formally the infinite representation (4.6) of W can be transformed into the infinite representation (4.10) by a "similarity" transformation. But this transformation is an unbounded operator. Concerning the many-time "matrix" representations, see appendix III.

5. The N.T.D.-Procedure

The truncation procedure suggested in section 4, is already known in field theory as the socalled N.T.D.-method. In this method one replaces the exact functional T_{ab} of (4.1) by the truncated functional

$$T_{ab}^N(x,y) := \sum_{n,m=0}^{N} \varphi_{ab}^N(n \mid m)\,\langle x\,y \mid f_{nm}\rangle\,. \quad (5.1)$$

Using the properties of the set $\mid f_{ke}\rangle$ and $\mid \Phi_{hj}\rangle$ discussed in appendix II, one easily recognizes, that T_N^{ab} is given equivalently by

$$T_{ab}^N(x,y) = \sum_{h,j=0}^{N} \chi_{ab}^N\,(h \mid j)\,\langle x, y \mid \Phi_{hj}\rangle \quad (5.2)$$

where the amplitudes are connected by

$$\chi_{ab}^N(h \mid j) = \sum_{n,m=0}^{N} c_{hn}^T\, c_{jm}^T\, \varphi_{ab}^N(n \mid m)\,. \quad (5.3)$$

In principle the N.T.D.-method gives no prescription which of the different representations (5.1) or (5.2) of the truncated functional T has to be used for actual calculation. So one has two possibilities for approximate calculations. Namely for T_{ab}^N in the representation (5.1) one obtains the truncated system

$$\sum_{n,m=0}^{N} (W_{hj,\,nm} - \omega_{ab}^N\delta_{hn}\,\delta_{jm})\,\varphi_{ab}^N(n \mid m) = 0\,, \quad (5.4)$$

while for T_{ab}^N in the representation (5.2) one obtains the set

$$\sum_{n,m=0}^{N} (H_{hj,\,nm} - \omega_{ab}^N(s)\,\delta_{hn}\,\delta_{jm})\,\chi_{ab}^N(n \mid m, s) = 0. \quad (5.5)$$

Because the operator in (5.5) is a symmetric one, we denote its eigenvalues $\omega_{ab}^N(s)$ and its eigenvectors by $\chi_{ab}^N(n \mid m, s)$ and call the representation (5.5) the symmetric N.T.D.-representation. In contrast to (5.5), (5.4) contains an unsymmetric operator, therefore we call (5.4) the unsymmetric N.T.D.-representation.

One should emphasize, that only the truncation procedure itself on T_{ab} gives equivalent representations (5.1) and (5.3). In calculating the $\varphi_{ab}^N(n \mid m)$

from (5.4) and $\chi_{ab}^{N}(n \mid m, s)$ from (5.55) one destroys this equivalence because the systems (5.4) and (5.5) are inequivalent, as is shown in section 7. Therefore as a second step in the complete definition of the N.T.D.-method, one has to explain, which of the truncated sets one has to prefer. In the conventional field theoretic form of the N.T.D.-method, the unsymmetrical representation is preferred. But stimulated by the numerical results of SCHWARTZ [11], who stressed the importance of having symmetrical systems, we investigate the symmetrical N.T.D.-representation. Using this representation a proof of convergence for the truncated equation is quite simple.

6. Proof of Convergence for the Symmetric N.T.D.-Representation

Here we prove the convergence of truncated symmetrical operators. We assume to have an eigenvalue equation for the symmetrical operator W

$$W \mid T\rangle = \omega \mid T\rangle . \tag{6.1}$$

Then we use an orthonormalized system of functions, say $\mid \psi_\varrho\rangle$ with

$$\langle \psi_\mu \mid \psi_\varrho\rangle = \delta_{\mu\varrho} . \tag{6.2}$$

We are allowed to interprete the indices μ and ϱ as symbols for a manyfold of indices. Our considerations then are still valid, especially of course for the truncated operators of section 5.

We now define the projection operators

$$P_N := \sum_{\mu=0}^{N} \mid \psi_\mu\rangle \langle \psi_\mu \mid . \tag{6.3}$$

Applying these operators, the truncated equation formally may be written

$$P_N W P_N \mid T_N\rangle =: W_N \mid T_N\rangle = \omega \mid T_N\rangle \tag{6.4}$$

where $P_N \mid T_N\rangle = \mid T_N\rangle$. Expanding $\mid T_N\rangle$ in a series of $\mid \psi_\varrho\rangle$ and projecting from the left with the states $\langle \psi_a \mid$ one obtains the matrix representation form of section 5. We now prove the following theorem:

If $\omega^{(k)}$ is an eigenvalue of W, there is in any circle around $\omega^{(k)}$ an eigenvalue of W_N, if N is sufficiently large; i. e. for any $r > 0$ exists a N_r, so that all resolvents $R_N(\omega) := (\omega - W_N)^{-1}$ possess a pole within this circle for $N > N_r$.

This of course means convergence of the sequence of eigenvalues for the truncated systems (6.4), because r can be chosen arbitrarily small.

To prove this theorem, we assume it to be wrong. In this case there exists a $r_0 > 0$ and a partial sequence N' so that $R_{N'}(\omega)$ is regular within the circle around $\omega^{(k)}$ with radius r_0. To show that this is impossible we consider for the exact eigenvalue $\omega^{(k)}$ with eigenvector $\mid T^k\rangle$

$$W \mid T^k\rangle = \omega^{(k)} \mid T^k\rangle \tag{6.5}$$

and

$$\langle T^k \mid T^k\rangle =: \| T^k \|^2 = 1 \tag{6.6}$$

the identity

$$\mid T^k\rangle = R_{N'}(\omega^{(k)}) \, (\omega^{(k)} - W_{N'}) \mid T^k\rangle \tag{6.7}$$

from which follows

$$1 = \| R_{N'}(\omega^{(k)}) \, (\omega^{(k)} - W_{N'}) \, T^k \| \leqq \| R_{N'}(\omega^{(k)}) \| \; \| (\omega^{(k)} - W_{N'}) \, T^k \| . \tag{6.8}$$

Assuming now, that within this circle of radius r_0 around $\omega^{(k)}$ there is no pole of $R_{N'}(\omega)$; there exists an estimate for the norm of the resolvent [13]

$$\| R_{N'}(\omega^{(k)}) \| \leqq r_0^{-1}. \tag{6.9}$$

But now (see appendix IV)

$$\lim_{N\to\infty} \| (\omega^{(k)} - W_{N'}) \, T^k \| = 0. \tag{6.10}$$

Therefore inserting (6.9) and (6.10) into (6.8) we find a contradiction, and so the convergence is proved.

Further for the special problem considered in section 5. The convergence of the eigenvectors of W can be proven too, if an additional assumption is made, which is indicated in the proof.

To show this we consider the relation (proved in appendix IV)

$$\lim_{N\to\infty} \| (\omega^{(k)} P_N - P_N W P_N) \, T^k \| = 0 . \tag{6.11}$$

If now $\mid T^k\rangle$ $(k = 1, \dots, N)$ are the eigenvectors of $P_N W P_N$ with eigenvalues $\omega_N^{(k)}$, then we may expand

$$P_N \mid T^k\rangle = \sum_{i=1}^{N} \langle T^k \, T_N{}^i\rangle \mid T_N{}^i\rangle \tag{6.12}$$

and

$$P_N W P_N \mid T^k\rangle = \sum_{i=1}^{N} \omega_N{}^i \langle T^k \, T_N{}^i\rangle \mid T_N{}^i\rangle . \tag{6.13}$$

Therefore

$$\| (\omega^{(k)} P_N - P_N W P_N) \, T^k \|^2 = (\omega^{(k)} - \omega_N^{(k)})^2 \langle T^k \, T_N^{(k)}\rangle^2 + \sum_{i \neq k}^{N} (\omega^{(k)} - \omega_N^{(i)})^2 \, \langle T^k \, T_N^{\,i}\rangle^2. \tag{6.14}$$

[13] FR. RIESZ and B. SZ. NAGY, Vorlesungen über Funktionalanalysis, VEB Verlag der Wissenschaften, Berlin 1956, S. 398.

Now we make the plausible assumption that for sufficiently large N

$$|\omega^{(k)} - \omega_N^{(i)}| \geqq a \tag{6.15}$$

for $i \neq k$, i. e. that only the sequence $\omega_N^{(i)}$ converges towards $\omega^{(k)}$ with

$$\lim_{N\to\infty} |\omega^{(k)} - \omega_N^{(k)}| = 0 . \tag{6.16}$$

Therefore it follows from (6.11) and (6.14), that for $i \neq k$

$$\lim_{N+\infty} \sum_{i \neq k} \langle T^k T_N{}^i \rangle^2 = 0 \tag{6.17}$$

has to be valid.

On the other hand it follows from the expansion (6.15) that

$$\sum_{i=1}^{N} \langle T^k T_N{}^i \rangle^2 = 1 . \tag{6.18}$$

So it follows together with (6.17) that

$$\lim_{N'\to\infty} \langle T^k T_N{}^k \rangle = 1 \tag{6.19}$$

with a suitably chosen phase factor of $|T_N^k\rangle$ and therefore that

$$\lim_{N\to\infty} \| (T^k - T_N{}^k) \|^2 = \lim_{N\to\infty} 2(1 - \langle T^k T_N{}^k \rangle) = 0 \tag{6.20}$$

i. e. convergence of the eigenvectors in the $|\psi_\mu\rangle$-representation.

7. Connection Between the Symmetric and the Unsymmetric N.T.D.-Representation

The unsymmetrical N.T.D.-representation (5.4) can be written as

$$\sum_{k,l=0}^{N} \langle h_{nm} W f_{kl} \rangle \, \varphi^N(k\,|\,l) = \omega \, \varphi^N(n\,|\,m) . \tag{7.1}$$

Using the expansions of appendix II, we have formally

$$\langle h_{nm} | = \sum_{s,r=0}^{\infty} d_{ns} \, d_{mr} \, \langle \Phi_{sr} | \tag{7.2}$$

and

$$| f_{kl} \rangle = \sum_{t,v=0}^{N} c_{kt} \, c_{lv} \, | \Phi_{tv} \rangle . \tag{7.3}$$

Substitution of (7.2) and (7.3) into (7.1) then gives

$$\sum_{k,l=0}^{N} \sum_{s,r,t,v=0}^{\infty} d_{ns} \, d_{mr} \, \langle \Phi_{sr} W \Phi_{tv} \rangle \, c_{tk}^T \, c_{ve}^T \, \varphi^N(k\,|\,l) = \omega \, \varphi^N(n\,|\,m) \tag{7.4}$$

where the upper index T means the transposed matrix. Now we multiply (7.4) by $c_{hn}^T \, c_{jm}^T$ and sum over $n, m = 0, \ldots, N$. Observing the orthonormality properties of the c^T and d matrices (see appendix II) and substituting the transformed state vector

$$\chi^N(h\,|\,j) := \sum_{n,m=0}^{N} c_{hn}^T \, c_{jm}^T \varphi^N(n\,|\,m) \tag{7.5}$$

we obtain, by using the relations

$$\sum_{k,l=0}^{N} c_{tk}^T \, c_{ve}^T \varphi^N(k\,|\,l) = 0, \quad v, t \in \mathfrak{R} \tag{7.6}$$

from (7.4), the equations

$$\sum_{t,v=0}^{N} (\langle \Phi_{hj} W \Phi_{tv} \rangle - \omega \, \delta_{ht} \, \delta_{jv}) \, \chi^N(t\,|\,v) = \sum_{n,m\in\mathfrak{R}} \sum_{s,r=0}^{\infty} \sum_{t,v=0}^{N} c_{hn}^T \, c_{jm}^T \, d_{ns} \, d_{mr} \, \langle \Phi_{sr} W \Phi_{tv} \rangle \, \chi^N(t\,|\,v) \tag{7.7}$$

where $\mathfrak{R}$ in (7.6) and in the first summation on the right hand side of (7.7) means summation over the complement set to $m, n = 0, \ldots, N$.

By the transformation of (7.1) into (7.7) it is shown that the truncated symmetric and unsymmetric N.T.D.-representations are inequivalent. The unsymmetric N.T.D.-representation appears as a perturbed symmetric N.T.D.-representation, where the perturbing operator is defined by the terms on the right hand side of (7.7). It might be, that the formulation (7.7) of the unsymmetric N.T.D.-representation can be used for a proof of convergence in this representation. But because the corresponding projection operators P_N are unbounded for all N, this entertainment is not very hopeful. The numerical values for the unsymmetrical representation, obtained so far and given in section 8, do also not support the attempt to prove convergence.

8. Numerical Results

For all numerical calculations, one has to change the double index n, m into one index, say r. But there is no unique correspondence between the grid numbers n, m and the line numbers r. The two, most obvious possibilities are the triangular and the square denumeration. For the triangular denumeration r runs along the diagonals of the grid n, m and for the square denumeration r runs along the squares of the grid n, m. This gives rise to two different truncation schemes

$$m + n \leqq N , \quad N = 1, 3, 5, \ldots \text{ (triangular)}$$

$$m \leqq N ; \quad n \leqq N , \quad N = 1, 2, \ldots \quad \text{(square)}$$

where the triangular truncated grid gives $\frac{1}{4}(N+1)(N+3)$ equations, while the square truncated grid gives $\frac{1}{2}(N+1)^2$ equations for T functions between states of different parity. By help of (1.3) it can be easily verified, that the triangular truncation is equivalent to the truncation used in spinor theory. In section 5 we used square truncation, but of course our arguments do not depend on a special truncation procedure. We used square truncation only for simplicity.

Our standards for comparison purposes, we get from calculations with ordinary SCHRÖDINGER theory. The HAMILTONIAN $H := \frac{1}{2}\, p^2 + \frac{1}{4}\, q^4$ belongs to the equation of motion (1.1). From this HAMILTONIAN one obtains by direct calculation, see ref. [7]

$$\omega_{01} = 1{,}0871, \quad \Delta = 0{,}4561, \quad \Gamma = 0{,}5611 .$$

We now compare this result firstly with the approximate eigenvalues of the symmetrical N.T.D.-representation. As we see in Fig. 1 and Fig. 2 the convergence proved in section 6 is quite good numerically. In Fig. 3 the convergence of the first component of the corresponding eigenvector is shown numerically. For the calculation of the unsymmetric N.T.D.-representation, we refer to the paper of SCHWARTZ [11]. His results can be seen in Fig. 4 and Fig. 5. Only the first values have been verified by our own calculations. Although the unsymmetric eigenvalues lie within some percentage around the exact eigenvalue, one cannot see a systematic approach, where the

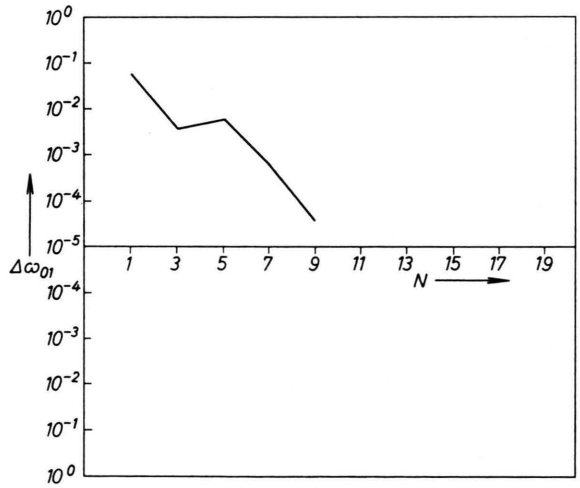

Fig. 1. Error $\Delta\omega_{01} := (\omega_{01}^N\,(s) - \omega_{01})$ as it depends on the truncation number N for the symmetric N.T.D.-representation and diagonal truncation. Values of Δ and Γ are 1/2. For $N > 9$ the limits of accuracy for the computer are reached.

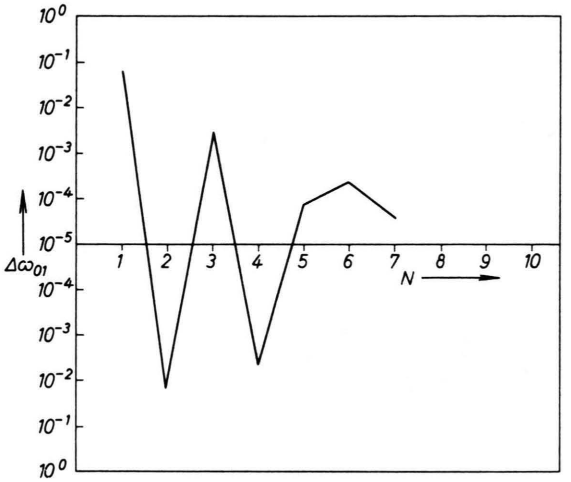

Fig. 2. Error $\Delta\omega_{01} := (\omega_{01}^N(s) - \omega_{01})$ as it depends on the truncation number N for the symmetric N.T.D.-representation and square truncation. Values of Δ and Γ are 1/2. For $N > 7$ the limits of accuracy for the computer are reached.

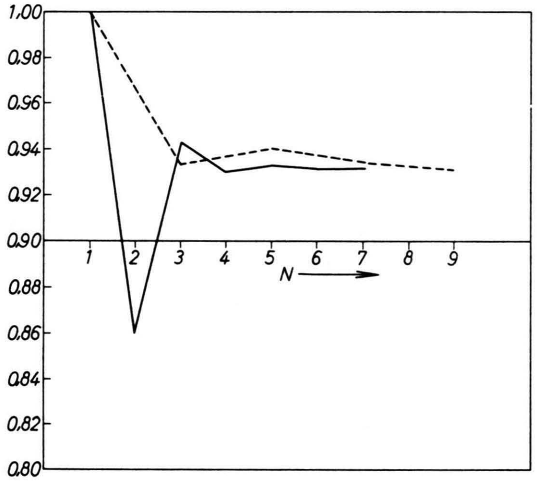

Fig. 3. Value of the first expansion coefficient for the truncated Φ-functions as it depends on the truncation number N for the symmetric N.T.D.-representation. Dotted lines indicate diagonal truncation, full lines, square truncation.

error becomes smaller and smaller. Assuming that the unsymmetric truncation makes sense at all, one can give a heuristical argument, explaining this behavior. Looking at the unsymmetric N.T.D.-representation as a superposition of a convergent truncated symmetric operator and a perturbation term according to section 7, one could imagine, that a rough measure of unsymmetric eigenvalue convergence is defined by the ratio between perturbed and unperturbed matrix elements for any truncation step N. Assuming that the number of unperturbed matrix

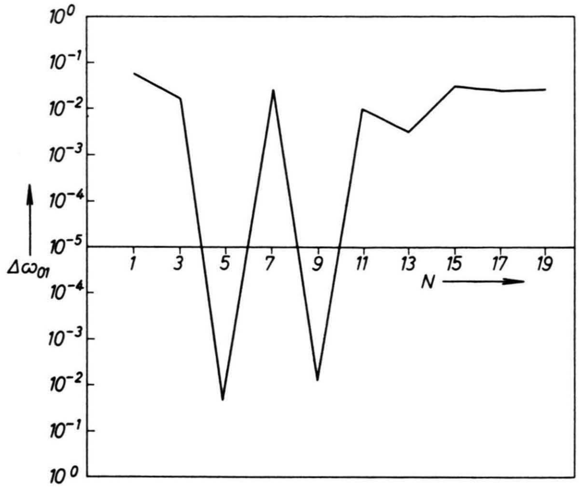

Fig. 4. Error $\Delta\omega_{01} := (\omega_{01}^{N}(s) - \omega_{01})$ as it depends on the truncation number N for the unsymmetric N.T.D.-representation and diagonal truncation according to SCHWARTZ. Values of Δ and Γ are 1/2.

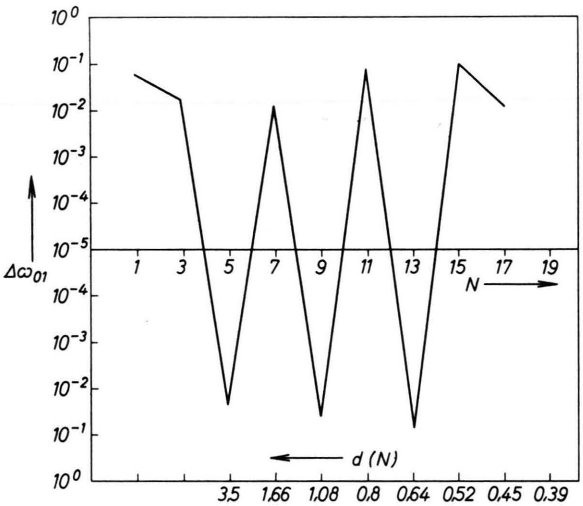

Fig. 5. Error $\Delta\omega_{01} := (\omega_{01}^{N}(s) - \omega_{01})$ as it depends on the truncation number N for the unsymmetric N.T.D.-representation and square truncation according to SCHWARTZ. Values of Δ and Γ are 1/2. Beneath, the corresponding ratio d(N) is given.

elements is much larger than the number of perturbed elements, one would expect, that the eigenvalues of the symmetric operator are nearly reproduced and therefore the N.T.D.-convergence becomes quite good. Defining d(N) as this ratio, one therefore has to keep $\mathrm{d}(N) \ll 1$ to assure good convergence. The number of perturbing matrix elements is according to (7.7) and Appendix II for odd N and square truncation equal to $(N+1)^2\,(3\,N-1)$ and therefore

$$\mathrm{d}(N) = \frac{(3\,N-1)}{\frac{1}{2}(N+1)^2 - (3\,N+1)}\,.$$

In Fig. 5 we write the d(N) ratios beneath the truncation numbers N. For $N=3$ all elements are perturbed and therefore in Fig. 5 the d(N) numbers start with $N=5$. Comparing these numbers with our postulate of convergence, one may understand the results of SCHWARTZ, and for getting better converging unsymmetrical N.T.D.-values one would have to carry out the calculations for values of N much larger than SCHWARTZ has done. For example to obtain a $\mathrm{d}(N) \approx 10^{-1}$ one has to put $N \approx 50$. Naturally in this region the practical calculations require an enormous amount of labour, because the number of unknowns then is very large. But we once more stress, that this consideration is speculative.

Acknowledgements

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Appendix I

The operator reads explicitly

$$\begin{aligned}\int j_\alpha(t)\, O_\alpha\left(j_1\, j_2\,, \frac{\mathrm{d}}{\mathrm{d}j_1}\, \frac{\mathrm{d}}{\mathrm{d}j_2}\right)\mathrm{d}t &= j_1 \cdot \frac{\delta}{\delta j_2} \\ &- (j_1 \cdot F_{22} \cdot j_2 + j_1 \cdot F_{21} \cdot j_1) + 3\,F_{11}(0)\,(j_2 \cdot F_{11} \cdot j_1 \\ &+ j_2 \cdot F_{12} \cdot j_2) - j_2 \cdot (F_{11} \cdot j_1 + F_{12} \cdot j_2)^3 - 3\,F_{11}(0)\; j_2 \cdot \frac{\delta}{\delta j_1} \\ &+ 3\, j_2 [\,(F_{11} \cdot j_1 + F_{12} \cdot j_2)^2 \cdot \frac{\delta}{\delta j_1} \\ &- 3\, j_2 \left[(F_{11} \cdot j_1 + F_{12} \cdot j_2) \cdot \frac{\delta^2}{\delta j_1{}^2}\right] + j_2 \cdot \frac{\delta^3}{\delta j_1{}^3}\end{aligned} \tag{I.1}$$

where we used the abbreviation

$$j_\alpha \cdot F_{\gamma\delta} \cdot j_\beta := \int j_\alpha(t)\; F_{\gamma\delta}(t-t')\; j_\beta(t')\;\mathrm{d}t\,\mathrm{d}t' \tag{I.2}$$

etc. It is

$$\begin{aligned} F_{11}(t) &= \langle 0\,|\,T\,q(t)\;q(0)\,|\,0\rangle\,, \\ F_{12}(t) &= \langle 0\,|\,T\,q(t)\;p(0)\,|\,0\rangle\,, \\ F_{21}(t) &= \langle 0\,|\,T\,p(t)\;q(0)\,|\,0\rangle\,, \\ F_{22}(t) &= \langle 0\,|\,T\,p(t)\;p(0)\,|\,0\rangle\,. \end{aligned} \tag{I.3}$$

Therefore it follows

$$F_{12}(t)+F_{21}(t)=0\,,\quad F_{12}(-t)=F_{21}(t),\quad F_{12}(-t)=-F_{12}(t), \tag{I.4}$$

$$F_{21}(-t)=-F_{21}(t), \tag{I.5}$$

and

$$j\cdot F_{12}\cdot j=j\cdot F_{21}\cdot j=0\,. \tag{I.6}$$

This firstly has to be observed for the evaluation of (I.1).

Further $F_{11}(t)$ and $F_{22}(t)$ are continuous functions with the limiting values $\Delta=F_{11}(0)$ and $\Gamma=F_{22}(0)$, whereas $F_{12}(t)$ and $F_{21}(t)$ are discontinuous functions, the limits of which are known. By these rules we are able to evaluate the limit of (I.1). It is for example

$$\mathrm{Lim}\; j_1\cdot F_{22}\cdot j_2=\Gamma\, x\, y \tag{I.7}$$

or

$$\mathrm{Lim}\; j_1\cdot \frac{\delta}{\delta j_2}=x\,\frac{\partial}{\partial y}\,. \tag{I.8}$$

On the other hand the more difficult terms are those containing F_{12}. There we get for example

$$j_2(F_{11}\,j_1)^2\,F_{12}\,j_2:=\int F_{11}(t_1-t_2)\;F_{11}(t_1-t_3)\; F_{12}(t_1-t_4)\;j_2(t_1)\;j_1(t_2)j_1(t_3)\;j_2(t_4)\;\mathrm{d}t_1\ldots\mathrm{d}t_4 \tag{I.9}$$

then

$$\mathrm{Lim}\; j_2(F_{11}\,j_1)^2\,F_{12}\,j_2= \frac{1}{4!}\sum_{\varepsilon_{i_1}>\ldots>\varepsilon_{i_4}}\lim_{\varepsilon_i\to 0}F_{11}(\varepsilon_{i1}-\varepsilon_{i2})\;F_{11}(\varepsilon_{i1}-\varepsilon_{i3})\; F_{12}(\varepsilon_{i1}-\varepsilon_{i4})\;x^2\,y^2$$

$$=\frac{3\,\Delta^2}{2!}\;[F_{12}(+0)+F_{12}(-0)]\,x^2\,y^2\neq 0\,. \tag{I.10}$$

Applying this procedure on each term of (I.1), we get

$$\mathrm{Lim}\int j_a(t)\;O_a\Big(j_1\,j_2\,,\,\frac{\mathrm{d}}{\mathrm{d}j_1}\,\frac{\mathrm{d}}{\mathrm{d}j_2}\Big)\,\mathrm{d}t$$

$$=x\frac{\partial}{\partial y}-\Gamma\,x\,y+3\,\Delta^2\,x\,y-\Delta^3\,x^3\,y +\tfrac{1}{4}\Delta x\,y^3-3\,\Delta y\,\frac{\partial}{\partial x}+3\,\Delta^2\,x^2\,y\,\frac{\partial}{\partial x} +\frac{1}{4}\,y^3\,\frac{\partial}{\partial x}-3\,\Delta x\,y\,\frac{\partial^2}{\partial x^2}+y\,\frac{\partial^3}{\partial x^3}$$

$$=:\mathfrak{W}\Big(x,y,\,\frac{\mathrm{d}}{\mathrm{d}x}\,\frac{\mathrm{d}}{\mathrm{d}y}\Big)\,. \tag{I.11}$$

Appendix II

We have

$$|\,h_{nm}\rangle\equiv|\,h_n\rangle\,|\,h_m\rangle \tag{II.1}$$

$$\langle x,y\,|\,f_{kl}\rangle\equiv f_{kl}(x,y)\equiv f_k(x)\;f_l(y) \tag{II.2}$$

with

$$f_k(x)\;:=\frac{1}{k!}\;x^k\exp-\Big(\frac{\Delta}{2}\,x^2\Big) \tag{II.3}$$

$$f_l(y)\;:=\frac{1}{l!}\;x^l\exp-\Big(\frac{\Gamma}{2}\,y^2\Big), \tag{II.4}$$

according to the definitions of section 3, namely (3.10) and (3.24). Further for the reciprocal basis vectors the relations

$$\langle h_n\,f_k\rangle=\delta_{nk}\,, \tag{II.5}$$

$$\langle h_m\,f_l\rangle=\delta_{ml} \tag{II.6}$$

are valid. — By definition we put

$$\langle x,y\,|\,\Phi_{rs}\rangle\;:=\;\Phi_{rs}(x,y)\;:=\;\Phi_r(x)\;\Phi_s(y) \tag{II.7}$$

where $\Phi_r(x)$ resp. $\Phi_s(y)$ are eigenfunction of the harmonic oscillator, defined by

$$\Phi_r(x)\;:=H_s(\sqrt{2\,\Gamma}\;y)\;\exp-\Big(\frac{\Delta}{2}\,x^2\Big), \tag{II.8}$$

$$\Phi_s(y)\;:=H_r(\sqrt{2\,\Delta}\;x)\;\exp-\Big(\frac{\Gamma}{2}\,y^2\Big) \tag{II.9}$$

where $H_n(\xi)$ is a normalized Hermitian polynomial.

Then the expansions

$$|\,h_n\rangle\;=\;\sum_{s=0}^{\infty}d_{ns}\,|\,\Phi_s\rangle\;\;(\text{formally}) \tag{II.10}$$

$$f_k(x)\;=\;\sum_{t=0}^{\infty}c_{kt}\;\Phi_t(x) \tag{II.11}$$

are possible. Expansions with the same coefficients exist for the y-functions

$$|\,h_m\rangle\;=\;\sum_{r=0}^{\infty}d_{mr}\,|\,\Phi_r\rangle\;\;(\text{formally}) \tag{II.12}$$

$$f_l(y)\;=\;\sum_{v=0}^{\infty}c_{lv}\;\Phi_v(y)\,. \tag{II.13}$$

It is

$$d_{ns}:=\;\langle h_n\,\Phi_s\rangle\,, \tag{II.14}$$

$$c_{kt}:=\;\langle f_k\,\Phi_t\rangle \tag{II.15}$$

and because of

$$\Phi_s(x)=\;\sum_{a=0}^{\infty}\;\gamma_a^s\,\Theta(s-a)\;f_a(x) \tag{II.16}$$

and of (II.5) we get

$$d_{ns}=\langle h_n\,\Phi_s\rangle=\gamma_n^s\;\Theta(s-n)\,. \tag{II.17}$$

According to standard formulas we have for $(s-n)$ even

$$d_{ns}=\frac{(-1)^{\frac{1}{2}(s-n)}\;\sqrt{s!}}{\sqrt[4]{2\,\pi}\;2^{\frac{1}{2}(s-n)}\;\Big(\frac{s-n}{2}\Big)!}\;\Theta(s-n)$$

$$\approx\text{const}\,\sqrt{\frac{s!}{(s-n)\,!}}\;\Theta(s-n) \tag{II.18}$$

for large s and n. Otherwise d_{ns} is equal to zero.

Further according to SCHMIDT's orthogonalisation procedure it follows from (II.16) that the reciprocal relation (II.11) has to have expansion coefficients of the form

$$c_{lm} = c_{lm}\,\Theta(l-m) \qquad \text{(II.19)}$$

and

$$c_{lm}^T = c_{ml}\,\Theta(m-l) \qquad \text{(II.20)}$$

with

$$c_{lm} := \sqrt[4]{2\pi}\,\frac{1}{\frac{l-m}{2}\,!\;2^{\frac{1}{2}(l-m)}\sqrt{m!}}$$

$$\approx \text{const}\,\frac{1}{\sqrt{(l-m)!\,m!}} \qquad \text{(II.21)}$$

for $(l-m)$ even. Otherwise c_{lm} is equal to zero.

From (II.5) follows by inserting (II.10), (II.11) and observing the orthonormality relations between the Φ_k

$$\delta_{nk} = \sum_{t=0}^{\infty} d_{nt}\,c_{kt} = \sum_{t=0}^{\infty} d_{nt}\,c_{tk}^T \qquad \text{(II.22)}$$

that means

$$d_{nt} \equiv (c^{T-1})_{nt}\,. \qquad \text{(II.23)}$$

These relations are sufficient to understand all operations of section 7, concerning the transformation to the Φ system (II.7).

To get the operator W in the representation (II.7) we define the matrices

$$D_{kl}^{\pm} := (\sqrt{j}\,\delta_{k,j-1} \pm \sqrt{j+1}\,\delta_{k,j+1}), \qquad \text{(II.24)}$$

$$F_{lm}^{\pm} := \sqrt{m(m-1)(m-2)}\,\delta_{l,m-3} \pm 3\,m\sqrt{m}\,\delta_{l,m-1} + 3(m+1)\sqrt{(m+1)}\,\delta_{l,m+1} \pm \sqrt{(m+1)(m+2)(m+3)}\,\delta_{l,m+3}. \qquad \text{(II.25)}$$

Then we get the symmetrical matrix representation of W as

$$\langle \Phi_{mn}\,W\,\Phi_{\mu\nu}\rangle := \frac{1}{2}\sqrt{\frac{\Gamma}{\Delta}}\,D_{m\mu}^{+}\,D_{n\nu}^{-} + \frac{\Delta}{4}\sqrt{\frac{\Delta}{\Gamma}}\,F_{m\mu}^{-}\,D_{m\nu}^{+} - \frac{1}{16\,\Gamma}\sqrt{\frac{\Delta}{\Gamma}}\,D_{m\mu}^{-}\,F_{n\nu}^{+}\,. \qquad \text{(II.26)}$$

The operator W in the unsymmetrical representation is given by

$$\langle h_{nm}\,W\,f_{kl}\rangle := m\,\delta_{n+3,m-1,kl} + 3\,\Delta m(n+1)\,\delta_{n+1,m-1,kl} - n\,\delta_{n-1,m+1,kl} - \tfrac{1}{4}m(m-1)(m-2)\,\delta_{n+1,m-3,kl} - (\Gamma - 3\,n\,\Delta^2)\,m\,n\,\delta_{n-1,m-3,kl} - \frac{\Delta}{4}\,n\,m(m-1)(m-2)\,\delta_{n-1,m-3,kl} + \Delta^3 n(n-1)(n-2)\,m\,\delta_{n-3,m-1,kl}\,. \qquad \text{(II.27)}$$

Appendix III

To obtain the many-time matrix representations, we interprete the WICK-rule (1.11) as an expansion for $\mathfrak{T}_{ab}(j_1\,j_2)$. Writing

$$\mathfrak{T}_{ab}(j_1\,j_2) = \sum_{n,m}\int \varphi_{ab}^{nm}(t_1\ldots t_n, t_1'\ldots t_m')\,|\,\mathfrak{f}_{nm}(t_1\ldots t_n, t_1'\ldots t_m')\,\rangle\,\mathrm{d}t_1\ldots\mathrm{d}t_m' \qquad \text{(III.1)}$$

we define the expansion functionals $|\,\mathfrak{f}_{nm}\rangle$ as

$$|\,\mathfrak{f}_{nm}(t_1\ldots t_n, t_1'\ldots t_m')\,\rangle := |\,f_{nm}(t_1\ldots t_n, t_1'\ldots t_m')\,\rangle \times \exp(-\tfrac{1}{2}j_\alpha\cdot F_{\alpha\beta}\cdot j_\beta) \qquad \text{(III.2)}$$

where the point means a scalar product, i. e. ordinary integration and $|\,f_{nm}\rangle$ is defined by

$$|\,f_{nm}(t_1\ldots t_n, t_1'\ldots t_m')\,\rangle := \frac{i^{n+m}}{n!\,m!}\,j_1(t_1)\ldots j_1(t_n)\,j_2(t_1')\ldots j_2(t_m')\,. \qquad \text{(III.3)}$$

The corresponding reciprocal set is defined by

$$\langle\,\mathfrak{P}_{nm}(t_1\ldots t_n, t_1'\ldots t_m')\,| := \langle\,p_{nm}(t_1\ldots t_n, t_1'\ldots t_m')\,|\exp\,j_\alpha\cdot F_{\alpha\beta}\cdot j_\beta \qquad \text{(III.4)}$$

with

$$\langle\,p_{nm}(t_1\ldots t_n, t_1'\ldots t_m')\,| := \frac{\delta^n}{i^n\,\delta j_1(t_1)\ldots\delta j_1(t_n)}\,\frac{\delta^m}{i^m\,\delta j_2(t_1')\ldots\delta j_2(t_m')} \qquad \text{(III.5)}$$

and the property

$$\langle\,\mathfrak{P}_{nm}(t_1\ldots t_n, t_1'\ldots t_m')\,\mathfrak{f}_{kl}(s_1\ldots s_k, s_1'\ldots s_k')\,\rangle = \delta_{nk}\,\delta_{ml}\,\delta(t_1-s_1)\ldots\,\delta(t_m'-s_m')\,. \qquad \text{(III.6)}$$

The "states" (III.4) and (III.5) can be used to project out the desired τ- and φ-functions from the functionals, and to derive corresponding equations for these functions. So we have

$$\tau_{nm}^{ab}(t_1\ldots t_n, t_1'\ldots t_m') = \langle\,p_{nm}(t_1\ldots t_n, t_1'\ldots t_m')\,\mathfrak{T}_{ab}(j_1\,j_2)\,\rangle \qquad \text{(III.7)}$$

and

$$\varphi_{nm}^{ab}(t_1\ldots t_n, t_1'\ldots t_m') = \langle\,p_{nm}(t_1\ldots t_n, t_1'\ldots t_m')\;\Phi_{ab}(j_1\,j_2)\,\rangle\,. \qquad \text{(III.8)}$$

The equations of motion are

$$\sum_{h,l,s,s}\langle\,p_{nm}(t_1\ldots t_n, t_1'\ldots t_m')\left[i\,\omega_{ab} - \int j_\alpha(t)\,O_\alpha\!\left(j_1\,j_2, \frac{\mathrm{d}}{\mathrm{d}j_1}\,\frac{\mathrm{d}}{\mathrm{d}j_2}\right)\mathrm{d}t\,\right]f_{kl}(s_1\ldots s_k, s_1'\ldots s_l')\,\rangle \times \langle\,p_{kl}(s_1\ldots s_s, s_1'\ldots s_l')\;\Phi_{ab}(j_1\,j_2)\,\rangle = 0 \qquad \text{(III.9)}$$

and it is

$$\operatorname{Lim}\,\mathfrak{P}_{nm}(t_1\ldots t_n, t_1'\ldots t_m') \equiv \langle\,h_{nm}\,| := \exp\!\left(\frac{\Delta}{2}x^2 + \frac{\Gamma}{2}y^2\right)\frac{1}{i^{n+m}}\,\delta^{(n)}(x)\,\delta^{(m)}(y) \quad (x=y=0)\,. \qquad \text{(III.10)}$$

The truncated functionals are

$$\Phi_{ab}^{N}(j_1 j_2) = \sum_{n,m=0}^{N} \int \varphi_{nm}^{N}(t_1 \dots t_n, t_1' \dots t_m') \, | f_{nm}(t_1 \dots t_n, t_1' \dots t_m') \rangle \, \mathrm{d}t_1 \dots \mathrm{d}t_m' \qquad \text{(III.11)}$$

and by applying the Lim operator on (III.9) we obtain the unsymmetrical representation (4.4). The same is true for the truncated operators. Besides the reciprocal set (III.4) and the original set (III.2) there exists an orthogonal set of expansion functionals, the so-called HERMITEAN functionals [14]. They should lead to symmetric problems. But no particular work has been done so far in this direction.

Appendix IV

We want to prove the statements (6.10) and (6.11) of the text. For this reason we at first prove the

Theorem: If H is a symmetric operator in HILBERT space and $|\Phi_n\rangle$ a system of normalized eigenvectors of H with eigenvalues λ_n ($\lambda_n \neq 0$); if further $|f\rangle$ is in the domain of the k^{th} power H^k of H, then

$$|\langle f | \Phi_n \rangle| \leqq \frac{N_k}{|\lambda_n{}^k|} \text{ with } N_k = \| H^k f \| < \infty$$

Proof: It is

$$\langle H^k f | \Phi_n \rangle = \lambda_n{}^k \langle f | \Phi_n \rangle \qquad \text{(IV.1)}$$

that gives

$$|\langle f | \Phi_n \rangle| = \frac{|\langle H^k f | \Phi_n \rangle|}{|\lambda_n|^k} \leqq \frac{\| H^k f \|}{|\lambda_n|^k} \text{ qued.} \qquad \text{(IV.2)}$$

Now let us choose $H := -\frac{1}{2}\,\mathrm{d}^2/\mathrm{d}x^2 + \frac{1}{2}\,x^2$ in $\mathfrak{L}^2$ and for $|\Phi\rangle$ the HERMITIAN functions $H_n(x)\exp(-\frac{1}{4}\,x^2)$. If $f(x)$ is a rapidly decreasing, infinitely often differentiable function, then for every k there exists a constant N_k

$$|\langle f \, \Phi_n \rangle| \leqq \frac{N_k}{n^k} \qquad \text{(IV.3)}$$

for all n.

The eigenfunctions $T_{ab}(x, y)$ of the operator W are of this type as can easily be seen from the connection with SCHRÖDINGER theory (3.5). That means, if we expand

$$|T^k\rangle = \sum_{m=0}^{\infty} \langle \Phi_m T_k \rangle \, | \Phi_m \rangle \qquad \text{(IV.4)}$$

then

$$\sum_{m=M}^{\infty} |\langle \Phi_m T^k \rangle|^2 = \|(1-P_M)\, T^k\|^2 \leqq \frac{N_l(k)}{M^l} \qquad \text{(IV.5)}$$

for some $N_l(k)$.

It follows

$$\begin{aligned} \|(\omega^{(k)} - W_{N'})\, T^k \| &= \|(1-P_{N'})\, W T^k + P_{N'} W (1-P_{N'})\, T^k \| \\ &\leqq |\omega^{(k)}| \, \|(1-P_{N'})\, T^k\| + \| P_{N'} W (1-P_{N'})\, T^k \| \\ &\leqq \frac{N_l(k)\,|\,\omega_k}{N'^l} + \left(\sum_{i=1}^{N'} \sum_{j>N'} \langle \Phi_i W \Phi_j \rangle \langle \Phi_j T^k \rangle |^2 \right)^{1/2} \\ &\leqq \frac{\text{const}\,(l,k)}{N'^{\,l-2}} \end{aligned} \qquad \text{(IV.6)}$$

because of $\quad |\langle \Phi_i W \Phi_j \rangle| \approx j^3.$

Therefore

$$\lim_{N' \to \infty} \|(\omega^{(k)} - W_{N'})\, T^k \| = 0 \,. \qquad \text{(IV.7)}$$

For the proof of (6.11) we observe that

$$\|(\omega^{(k)} P_N - P_N W P_N)\, T^k \| \leqq \|(\omega^{(k)} - W P_N)\, T^k \| \,. \qquad \text{(IV.8)}$$

Then we conclude as before

$$\lim_{N \to \infty} \|(\omega^{(k)} P_N - P_N W P_N)\, T^k \| = 0 \,. \qquad \text{(IV.9)}$$

[14] J. FRIEDRICHS and A. SHAPIRO, Seminar on Integr. of Functionals, New York University.