Many-Body-Systems and Exciton Model in New-Tamm-Dancoff-Formulation

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The NTD-method is a procedure to compute differences of eigenvalues in quantum mechanical problems: $\omega_{\alpha\beta}=\lambda_\alpha-\lambda_\beta$.

It is an instruction to transform and truncate an infinite linear system of eigenvalue equations $\omega\,\tau^k=\sum_m A^k{}_m\,\tau^m$ which is derived with the aid of fundamental field equations or corresponding Hamilton-operators, as e.g. with Heisenberg's nonlinear spinor equation. In this paper we want to test the NTD-method for a many-body-model in solid state physics. We elaborate on the physical and mathematical aspects by choosing a suitable transformation $\tau\to\varphi=C\,\tau$ to get a new linear system $\omega\,\varphi^k=\sum_{i=-2}^{1} B^k{}_{k+2i}\,\varphi^{k+2i}$ which permits a truncation to evaluate approximation of states.

The efficiency of this method is demonstrated by treating a two-body-system in presence of polarisation quanta, known as exciton model.

During the last years the New-Tamm-Dancoff-method (NTD-method) was used to compute elementary particle states in Heisenberg's nonlinear spinor theory [1]. In that procedure, however, one encounters some mathematical and physical problems, which can be demonstrated with the aid of quantum mechanical and field theoretical models. This was done in full length in the case of the unharmonic oscillator [2]. It seems to be useful to apply the NTD-method to nonrelativistic many-body-problems in solid state physics. So far most of these models have been evaluated with known quantum mechanical methods. We now want to compare these with the corresponding states inNTD-formalism. This may be a first step to obtain a depper understanding of the physical as well as the mathematical problems involved, in particular, since NTD is connected with non-selfadjoint but unbounded operators of a type, which have not yet been investigated by the mathematicians.

We define: A NTD-system for many-body-problems is an infinite system of coupled differential or integral equations for computing energy differences

$$\omega_{\alpha\beta}=E_\alpha-E_\beta\,.$$

In field theoretical formulation, for instance, it connects the so-called τ-functions [3]

$$\tau^k{}_{\alpha\beta}(x_1\ldots x_k)=\langle\alpha\,|\,T\,\psi(x_1)\ldots\psi(x_n)\cdot\psi^*(x_{n+1})\ldots\psi^*(x_k)\,|\,\beta\rangle$$

with each other.

($|\,\alpha\rangle$ and $|\,\beta\rangle$ are eigenstates of the problem, ψ and ψ^* are field operators and T is a time-ordering operator.) This "τ-system" arises with the aid of a fundamental field equation, or the corresponding Hamilton operator, and has the symbolical form

$$\omega\,\tau^k=A^k{}_{k+2}\,\tau^{k+2}+A^k{}_k\,\tau^k+A^k{}_{k-2}\,\tau^{k-2}.$$

This infinite system is linear, in contrast to the method of Green's-functions, but it is not possible to truncate the system to generate a finite one, which might be suited to performing approximations of physical states. Only an appropriate linear transformation, the so-called φ-transformation, permits finally such a truncation. Therefore we give a second definition:

NTD-method is an instruction to handle the τ-system, before a truncation is introduced. It has the form of Wick's normal-ordering relative to a groundstate specifying the proper inequivalent representation.

In solid state physics this concept allows a clear physical interpretation. For the electronic part we are able to give a formulation in analogy to nonlinear spinor theory, but without the problems of relativistic invariance. Now we can work on familiar ground of known solid state models. Especially the exciton and the electronic polaron model are appropriate to demonstrate the physical and mathematical problems connected with the NTD-method. For that reason we introduce an approximation for the exciton, suited to compare it with the ansatz of Haken's exciton model [4].

§ 1. The Hamiltonian in the Hermitean Field Operators

We begin with the Hamiltonian

$$\mathfrak{H}=\int \varphi^{+}(\boldsymbol{r})\left[-\frac{\hbar^2}{2m}\Delta_{\boldsymbol{r}}+\sum_f \frac{e\,e_f}{|\boldsymbol{r}-\boldsymbol{R}_f|}\right]\varphi(\boldsymbol{r})\,\mathrm{d}\tau + \tfrac{1}{2}\iint \varphi^{+}(\boldsymbol{r}_1)\varphi^{+}(\boldsymbol{r}_2)\,\frac{e^2}{|\boldsymbol{r}_1-\boldsymbol{r}_2|}\,\varphi(\boldsymbol{r}_2)\varphi(\boldsymbol{r}_1)\,\mathrm{d}\tau_1\,\mathrm{d}\tau_2 \tag{1.1}$$

which gives a description of a non-relativistic Fermi field in the potential of charged nuclei at the lattice points $\boldsymbol{R}_f$. The electronic field $\varphi(\boldsymbol{r})$ may be expanded in one-electron-functions $w_{\boldsymbol{m}i}(\boldsymbol{r})$ localized at the lattice points $\boldsymbol{m}$ and denoted by quantum numbers i, which describes, e. g. energybands

$$\varphi(\boldsymbol{r})=\sum_{\boldsymbol{m}i} w_{\boldsymbol{m}i}(\boldsymbol{r})\,\psi_{\boldsymbol{m}i}=\sum_{\boldsymbol{m}} \boldsymbol{w}^{\mathrm{T}}_{\boldsymbol{m}}(\boldsymbol{r})\cdot\boldsymbol{\psi}_{\boldsymbol{m}} \tag{1.2}$$

$\boldsymbol{w}^{\mathrm{T}}_{\boldsymbol{m}}(\boldsymbol{r})$ is a row vector consisting of the functions $w_{\boldsymbol{m}i}(\boldsymbol{r})$. $\boldsymbol{w}^{\#}_{\boldsymbol{m}}(\boldsymbol{r})=[\boldsymbol{w}^{+}_{\boldsymbol{m}}(\boldsymbol{r})]^{\mathrm{T}}$ is the corresponding column vector of the complex conjugate functions $w^{*}_{\boldsymbol{m}i}(\boldsymbol{r})$. $\psi_{\boldsymbol{m}i}$, $\psi^{*}_{\boldsymbol{m}i}$ are destruction and creation operators which satisfy the anticommunication relations

$$\{\boldsymbol{\psi}_{\boldsymbol{m}j},\ \psi^{+}_{\boldsymbol{n}i}\}=\delta_{\boldsymbol{m},\boldsymbol{n}}\,\delta_{i,j}\,. \tag{1.3}$$

The one-electron-functions may be atom- or Wannier functions

$$w_{\boldsymbol{m}i}(\boldsymbol{r})=v_{\boldsymbol{m}i}(\boldsymbol{r}-\boldsymbol{m}). \tag{1.4}$$

Spin variables are neglected. We will also omit those functions which characterize the continous spectrum. Hence there remains only a finite or a countable infinite set of quantum numbers i. The special form of these functions is object of later discussions.

The ansatz (1.2) inserted into (1.1) describes a many-electron-problem in a crystal, where the lattice coordinates are only parameters in the electronic part and where attention is directed towards the local properties of the crystal, e. g. to a perturbated ionic crystal. The use of Wannier functions, in the case of an ideal crystal is identical with a description by Bloch-functions. The Hamiltonian in matrixform is

$$\mathfrak{H}=\sum_{\boldsymbol{m}\boldsymbol{m}'}\psi^{+}_{\boldsymbol{m}}H_{\boldsymbol{m}\boldsymbol{m}'}\psi_{\boldsymbol{m}'}+\sum_{\substack{\boldsymbol{m}\boldsymbol{m}'\\ \boldsymbol{n}\boldsymbol{n}'}}\psi^{+}_{\boldsymbol{m}}\psi^{+}_{\boldsymbol{n}}\,W_{\boldsymbol{m}\boldsymbol{n}\boldsymbol{n}'\boldsymbol{m}'}\,\psi_{\boldsymbol{n}'}\psi_{\boldsymbol{m}'} \tag{1.5}$$

with matrixelements

$$H_{\boldsymbol{m}\boldsymbol{m}'}=\int \boldsymbol{w}^{\#}_{\boldsymbol{m}}(\boldsymbol{r})\left(-\frac{\hbar^2}{2m}\Delta_{\boldsymbol{r}}+\sum_f\frac{e\,e_f}{|\boldsymbol{r}-\boldsymbol{R}_f|}\right)\boldsymbol{w}^{\mathrm{T}}_{\boldsymbol{m}'}(\boldsymbol{r})\,\mathrm{d}\tau \tag{1.6}$$

and

$$W_{\boldsymbol{m}\boldsymbol{n}\boldsymbol{n}'\boldsymbol{m}'}=\tfrac{1}{2}\iint A_{\boldsymbol{m}\boldsymbol{m}'}(\boldsymbol{r}_1)\,\frac{e^2}{|\boldsymbol{r}_1-\boldsymbol{r}_2|}\,A_{\boldsymbol{n}\boldsymbol{n}'}(\boldsymbol{r}_2)\,\mathrm{d}\tau_1\,\mathrm{d}\tau_2\,. \tag{1.7}$$

Here $A_{\boldsymbol{m}\boldsymbol{m}'}(\boldsymbol{r})$ is the matrix

$$A_{\boldsymbol{m}\boldsymbol{m}'}(\boldsymbol{r})=\boldsymbol{w}^{\#}_{\boldsymbol{m}}(\boldsymbol{r})\,\boldsymbol{w}_{\boldsymbol{m}'}(\boldsymbol{r})=(w^{*}_{\boldsymbol{m}i}(\boldsymbol{r})\,w_{\boldsymbol{m}'j}(\boldsymbol{r}))\,. \tag{1.8}$$

In particular, the properties of Fermi operators demand for the components of (1.7) specially

$$W_{\boldsymbol{m}i,\boldsymbol{m}i,\boldsymbol{n}'l,\boldsymbol{m}'k}=0;\quad W_{\boldsymbol{m}i,\boldsymbol{n}j,\boldsymbol{n}'l,\boldsymbol{n}'l}=0\,. \tag{1.9}$$

It is useful to construct Hermitean operators[5]

$$\hat{\boldsymbol{\psi}}^{+}_{\boldsymbol{m}}=\hat{\boldsymbol{\psi}}^{\mathrm{T}}_{\boldsymbol{m}} \tag{1.10}$$

by doubling the components

$$\hat{\boldsymbol{\psi}}_{\boldsymbol{m}}=U^{+}\begin{pmatrix}\boldsymbol{\psi}_{\boldsymbol{m}}\\ \boldsymbol{\psi}^{\#}_{\boldsymbol{m}}\end{pmatrix},\qquad \{\hat{\psi}_{\boldsymbol{m}k},\ \hat{\psi}_{\boldsymbol{m}l}\}=\delta_{\boldsymbol{m},\boldsymbol{n}}\,\delta_{k,l}\,. \tag{1.11}$$

U is a unitary matrix

$$U=\frac{1}{\sqrt{2}}\begin{pmatrix}1 & i\\ 1 & -i\end{pmatrix}. \tag{1.12}$$

Now we also must double the Hamiltonian. Since the symmetric part of a matrice vanish in an antisymmetric formulation of the whole problem, we will construct only antisymmetric terms. Then we can verify the following expression

$$\mathfrak{H}=\tfrac{1}{2}\sum_{\boldsymbol{m}\boldsymbol{m}'}\hat{\psi}^{\mathrm{T}}_{\boldsymbol{m}}(\hat{H}_{\boldsymbol{m}\boldsymbol{m}'}+\hat{B}_{\boldsymbol{m}\boldsymbol{m}'})\hat{\psi}_{\boldsymbol{m}'} + \tfrac{1}{4}\sum_{\substack{\boldsymbol{m}\boldsymbol{m}'\\ \boldsymbol{n}\boldsymbol{n}'}}\hat{\psi}^{\mathrm{T}}_{\boldsymbol{m}}\,\hat{\psi}^{\mathrm{T}}_{\boldsymbol{n}}\,\hat{W}_{\boldsymbol{m}\boldsymbol{n}\boldsymbol{n}'\boldsymbol{m}'}\,\hat{\psi}_{\boldsymbol{n}'}\,\hat{\psi}_{\boldsymbol{m}'}+C \tag{1.13}$$

with

$$\begin{aligned}\hat{H}_{\boldsymbol{m}\boldsymbol{m}'}+\hat{B}_{\boldsymbol{m}\boldsymbol{m}'}&=U^{+}\begin{pmatrix}(H+B)_{\boldsymbol{m}\boldsymbol{m}'} & 0\\ 0 & (H+B)^{\mathrm{T}}_{\boldsymbol{m}\boldsymbol{m}'}\end{pmatrix}U\\ &=U^{\mathrm{T}}\begin{pmatrix}0 & -(H+B)^{\mathrm{T}}_{\boldsymbol{m}\boldsymbol{m}'}\\ (H+B)_{\boldsymbol{m}\boldsymbol{m}'} & 0\end{pmatrix}U\\ &=-(\hat{H}^{\mathrm{T}}_{\boldsymbol{m}\boldsymbol{m}'}+B^{\mathrm{T}}_{\boldsymbol{m}\boldsymbol{m}'}),\end{aligned} \tag{1.14}$$

$$\hat{W}_{\boldsymbol{m}\boldsymbol{n}\boldsymbol{n}'\boldsymbol{m}'}=\tfrac{1}{2}\iint \hat{A}_{\boldsymbol{m}\boldsymbol{m}'}(\boldsymbol{r}_1)\,\frac{e^2}{|\boldsymbol{r}_1-\boldsymbol{r}_2|}\hat{A}_{\boldsymbol{n}\boldsymbol{n}'}(\boldsymbol{r}_2)\,\mathrm{d}\tau_1\,\mathrm{d}\tau_2\,,$$

$$\hat{A}_{\boldsymbol{m}\boldsymbol{m}'}(\boldsymbol{r})=U^{+}\begin{pmatrix}A_{\boldsymbol{m}\boldsymbol{m}'}(\boldsymbol{r}) & 0\\ 0 & -A^{\mathrm{T}}_{\boldsymbol{m}\boldsymbol{m}'}(\boldsymbol{r})\end{pmatrix}U, \tag{1.15}$$

where

$$A^{\mathrm{T}}_{\boldsymbol{m}\boldsymbol{m}'}(\boldsymbol{r})=\boldsymbol{w}_{\boldsymbol{m}}(\boldsymbol{r})\,\boldsymbol{w}^{+}_{\boldsymbol{m}'}(\boldsymbol{r})=(w_{\boldsymbol{m}i}(\boldsymbol{r})\,w^{*}_{\boldsymbol{m}'j}(\boldsymbol{r}))\,, \tag{1.16}$$

$$B_{mm'} = \tfrac{1}{2}\iint \sum_{n} [A_{mm'}(\boldsymbol{r}_1)\,\mathrm{Tr}\,(A_{nn}(\boldsymbol{r}_2)) - A_{mn}(\boldsymbol{r}_1)A_{nm'}(\boldsymbol{r}_2)]\,\frac{e^2}{|\boldsymbol{r}_1-\boldsymbol{r}_2|}\,\mathrm{d}\tau_1\,\mathrm{d}\tau_2\,, \quad (1.17)$$

$$C = \tfrac{1}{2}\sum_{m}\mathrm{Tr}(H_{mm}) + \tfrac{1}{8}\sum_{mn}\iint \mathrm{Tr}\,(A_{mm}(\boldsymbol{r}_1))\,\frac{e^2}{|\boldsymbol{r}_1-\boldsymbol{r}_2|} \cdot \mathrm{Tr}\,(A_{nn}(\boldsymbol{r}_2))\,\mathrm{d}\tau_1\,\mathrm{d}\tau_2\,, \quad (1.18)$$

and
$$\mathrm{Tr}\,(A_{nn}(\boldsymbol{r})) = \sum_{i} w^{*}_{ni}(\boldsymbol{r})\,w_{n,i}(\boldsymbol{r}). \quad (1.19)$$

§ 2. A Functional-equation and the τ-System

The New-Tamm-Dancoff-method (NTD) was invented to compute energy differences. For this purpose we define the generating functional

$$\mathfrak{V} = e^{iC} := \sum_{n}\frac{i^n}{n!}C^n\,,\quad C = \sum_{\boldsymbol{p}}\hat{\boldsymbol{u}}^{\mathrm{T}}_{\boldsymbol{p}}\cdot\hat{\psi}_{\boldsymbol{p}} \quad (2.1)$$

where the $\hat{\boldsymbol{u}}_{\boldsymbol{p}}$ are vector variables with the folowing anticommutation relations for their components

$$\{\hat{u}_{pi}\,,\hat{u}_{qj}\} = 0;\quad \{\hat{u}_{pi}\,,\hat{\psi}_{qj}\} = 0 \quad \text{for all } \boldsymbol{p} \text{ and } i,\ \boldsymbol{q} \text{ and } j. \quad (2.2)$$

Moreover, we use operators $\hat{\partial}_{\boldsymbol{p}}$ with the properties [6]

$$\{\hat{\partial}_{pi}\,,\hat{u}_{qj}\} = \delta_{p,q}\delta_{i,j};\ \{\hat{\partial}_{pi},\hat{\psi}_{qj}\} = 0,\ \ \hat{\partial}_{\boldsymbol{p}}|\,0) = 0\,. \quad (2.3)$$

Here is $|\,0)$ the vacuum in U-space and the operators $\hat{\boldsymbol{u}}_{\boldsymbol{p}}$ and $\hat{\partial}_{\boldsymbol{p}}$ are non-Hermitean operators which anticommute with all $\hat{\psi}_{\boldsymbol{p}}$ [3]. With $\mathfrak{V}$ and the eigenstates $|\,\alpha\rangle$ and $|\,\beta\rangle$ we form the commutator

$$\langle\alpha|[\mathfrak{H},\mathfrak{V}]|\,\beta\rangle = (E_\alpha - E_\beta)\,\langle\alpha|\,\mathfrak{V}\,|\,\beta\rangle = \omega_{\alpha\beta}\,\langle\alpha|\,\mathfrak{V}\,|\,\beta\rangle\,. \quad (2.4)$$

The computation of the left-hand side can conventionally be achieved with the help of

$$[\mathfrak{H},\mathfrak{V}]|\,0) = \mathfrak{F}(\hat{\boldsymbol{u}},\hat{\partial})\mathfrak{V}\,|\,0) \quad (2.5)$$

which may be established with the relations

$$e^{iC}\hat{\varphi}_{\boldsymbol{m}}e^{-iC} = \sum_{n}\frac{1}{n!}\,[i\,C,[i\,C,[\ldots[i\,C,\hat{\psi}_{\boldsymbol{m}}]]\ldots] = \hat{\psi}_{\boldsymbol{m}} + i\,\hat{\boldsymbol{u}}_{\boldsymbol{m}} \quad (2.6)$$

and
$$\hat{\partial}_{\boldsymbol{m}}\,\mathfrak{V}\,|\,0) = (i\,\hat{\boldsymbol{\psi}}_{\boldsymbol{m}} - \tfrac{1}{2}\,\hat{\boldsymbol{u}}_{\boldsymbol{m}})\mathfrak{V}\,|\,0)\,. \quad (2.7)$$

Since
$$\mathrm{Tr}(\hat{A}_{\boldsymbol{nn}}) = \mathrm{Tr}(\hat{H}_{\boldsymbol{nn}}) = \mathrm{Tr}(\hat{B}_{\boldsymbol{nn}}) = 0 \quad (2.8)$$

holds, we find after some further steps

$$\mathfrak{F}(\hat{\boldsymbol{u}},\hat{\partial})\mathfrak{V}\,|\,0) = \{-\sum_{\boldsymbol{mm'}}\hat{\boldsymbol{u}}^{\mathrm{T}}_{\boldsymbol{m}}(\hat{H}_{\boldsymbol{mm'}} + \hat{B}_{\boldsymbol{mm'}})\,\hat{\partial}_{\boldsymbol{m'}} + \sum_{\substack{\boldsymbol{mm'}\\ \boldsymbol{nn'}}}(\hat{\boldsymbol{u}}^{\mathrm{T}}_{\boldsymbol{m}}\,\partial^{\mathrm{T}}_{\boldsymbol{n}}\,\hat{W}_{\boldsymbol{mnn'm'}}\,\hat{\partial}_{\boldsymbol{n'}}\,\hat{\partial}_{\boldsymbol{m'}} + \tfrac{1}{4}\hat{\boldsymbol{u}}^{\mathrm{T}}_{\boldsymbol{m}}\hat{\boldsymbol{u}}^{\mathrm{T}}_{\boldsymbol{n}}\hat{W}_{\boldsymbol{mnn'm'}}\,\hat{u}_{\boldsymbol{n'}}\,\hat{\partial}_{\boldsymbol{m'}})\}\mathfrak{V}\,|\,0). \quad (2.9)$$

The τ-system is a system of matrix equations resulting from (2.4), (2.5) and (2.9) by comparing the powers of $\hat{\boldsymbol{u}}^{\mathrm{T}}_{\boldsymbol{p}}$. For that reason we define

$$\langle\alpha|\,\mathfrak{V}\,|\,\beta\rangle = \sum_{n=0}^{\infty}\frac{i^n}{n!}\sum_{\boldsymbol{p}_1\ldots\boldsymbol{p}_n}\hat{\boldsymbol{u}}^{\mathrm{T}}_{\boldsymbol{p}_n}\hat{\boldsymbol{u}}^{\mathrm{T}}_{\boldsymbol{p}_{n-1}}\ldots\hat{\boldsymbol{u}}^{\mathrm{T}}_{\boldsymbol{p}_1}\hat{\tau}^{n}_{\alpha\beta}(\boldsymbol{p}_1\,\boldsymbol{p}_2\ldots\boldsymbol{p}_n) \quad (2.10)$$

with the so-called τ-functions

$$\hat{\tau}^{n}_{\alpha\beta}(\boldsymbol{p}_1\ldots\boldsymbol{p}_n) = \langle\alpha|\,\frac{1}{n!}\sum_{\lambda_1\ldots\lambda_n}(-1)^{P}\hat{\boldsymbol{\psi}}_{\boldsymbol{p}\lambda_1}\hat{\boldsymbol{\psi}}_{\boldsymbol{p}\lambda_2}\cdots\hat{\boldsymbol{\psi}}_{\boldsymbol{p}\lambda_n}|\,\beta\rangle\,. \quad (2.11)$$

They are antisymmetrical in all arguments. The τ's are vector components that belong to the basis vectors $\hat{\boldsymbol{u}}^{\mathrm{T}}_{\boldsymbol{p}_n}\ldots\hat{\boldsymbol{u}}^{\mathrm{T}}_{\boldsymbol{p}_1}|\,0)$. The right-hand side of (2.11) consists of the sum of all permutations of $\hat{\boldsymbol{\psi}}_{\boldsymbol{p}_1}\ldots\hat{\boldsymbol{\psi}}_{\boldsymbol{p}_n}$.

We compare the coefficients simply by operating of $(0|\prod_{i=1}^{k}\partial_{\boldsymbol{n}_i}$ onto (2.5) from the left after multiplication with $\langle\alpha|$ and $|\,\beta\rangle$. Thus, we obtain the matrix system

$$\omega_{\alpha\beta}\hat{\tau}^{k}_{\alpha\beta}(\boldsymbol{n}_1\ldots\boldsymbol{n}_k) = \sum_{i=1}^{k}\sum_{\boldsymbol{nn'm'}}\hat{W}_{\boldsymbol{n}_i\boldsymbol{nn'm'}}\cdot\hat{\tau}^{k+2}_{\alpha\beta}(\boldsymbol{n}_1\ldots\boldsymbol{m'}/i\ldots\boldsymbol{n}_k\boldsymbol{n'}\,\boldsymbol{n}) - \sum_{i=1}^{k}\sum_{\boldsymbol{m'}}(\hat{H}_{\boldsymbol{n}_i\boldsymbol{m'}} + \hat{B}_{\boldsymbol{n}_i\boldsymbol{m'}})\,\hat{\tau}^{k}_{\alpha\beta}(\boldsymbol{n}_1\ldots\boldsymbol{m'}/i\ldots\boldsymbol{n}_k) + \sum_{ij'}{}'\sum_{\boldsymbol{m'}}\hat{W}_{\boldsymbol{n}_i\boldsymbol{n}_j\boldsymbol{m'}}\,(-1)^{Pjj'}\cdot\hat{\tau}^{k-2}_{\alpha\beta}(\boldsymbol{n}_1\ldots\boldsymbol{m'}/i\ldots1/j\ldots1/j'\ldots\boldsymbol{n}_k). \quad (2.12)$$

Here the symbol $\boldsymbol{m'}/i$ means that in the position i the argument $\boldsymbol{n}_i$ will be replaced by $\boldsymbol{m'}$. Further the $1/j$ and $1/j'$ stands for "defect operators", which point out that the j-th and the j'th arguments are absent. Connected with this property is a sign $(-1)^{Pjj'}$, which is determined by the number of permutations necessary to displace the defect operators $1/j$ and $1/j'$ from the first and second position to the j-th and the j'-th position, respectively.

(2.12) is a linear eigenwertproblem. The NTD-method means the truncation of such a system at a number $k = N$ to compute approximations from

the resulting N-dimensional part of the system. A serious problem is the question whether such a truncation process leads to physical interesting results. Even if this is so, the importance of this method depends on the possibility to work with small N's to elaborate the physical relevant approximations. Otherwise the complexity of the truncated system prevents us from doing any calculation. From investigations with the anharmonic oscillator there exists some experience with this method. One can demonstrate that a linear transformation, the so-called φ-transformation, is necessary to obtain physical results. In our case, this φ-transformation has a physical meaning, too, and we understand this by discussing the matrix elements of the lowest order equations which arise succesively from the truncating of the transformed system. By this process we obtain informations not only about physical, but also about mathematical problems of the NTD-method.

§ 3. The φ-Transformation

The meaning of the "τ-functions" is a set of probability-amplitudes for manybody systems, or more precisely, bilinear combinations of such amplitudes. We can demonstrate this by a normal-ordering, which orders the creation parts in $\hat{\psi}$ to the left and the destruction parts to the right in (2.11). An analysis shows that in order to compute a many body problem, one needs an N comparable with the whole number of electrons in the crystal. Therefore, a computation of energy differences between excited states and the groundstate of the crystal is practically impossible. A better standpoint is the begin with an approximation for a real crystal, represented by filled valence bands, and the subsequent computation of energy differences between excited states and such an approximated groundstate. This groundstate is automatically improved in higher order approximations. We obtain such a situation by normal-ordering the operators in (2.11) relative to that approximated groundstate as a physical vacuum. For this reason we define projection operators Λ_p^V and Λ_p^L for all lattice points $\boldsymbol{p}$. The Λ_p^V picks out the n_p one-electron-functions $w_{pi}(\boldsymbol{r})$ which belong to the valence bands, and Λ_p^L the m_p functions, which belong to the conduction bands. They have the form

$$\Lambda_p^V = \begin{pmatrix} 1 & & & & \\ & \ddots & & & \\ & & 1 & & \\ & & & 0 & \\ & & & & \ddots \\ & & & & & 0 \end{pmatrix} \Big\} n_p = \text{number of electrons which belongs to the valence bands,}$$

$$\Lambda_p^L = \begin{pmatrix} 0 & & & & \\ & \ddots & & & \\ & & 0 & & \\ & & & 1 & \\ & & & & \ddots \\ & & & & & 1 \end{pmatrix} \Big\} m_p = \text{number of electrons which belongs to the conduction bands.} \tag{3.1}$$

It have

$$\Lambda_p^V + \Lambda_p^L = I;\ \Lambda_L^V \Lambda_p^L = \Lambda_p^L \Lambda_p^V = 0;$$
$$\Lambda_p^V \Lambda_p^V = \Lambda_p^V;\ \Lambda_p^L \Lambda_p^L = \Lambda_p^L. \tag{3.2}$$

Of course, this decomposition in Λ_p^V and Λ_p^L is not the only possible one. For particular lattice points, e. g. in perturbated areas of the crystal, we are able to make another decomposition. However, the former point of view is useful in the case of an ideal crystal. Here the choice of Wannier-functions for the localized w_{pi} allows the change to Bloch-functions, if it becomes necessary.

The normal-ordering is most easily arranged in the generating functional (2.1) with the aid of formula

$$e^{i(A+B)} = e^{\frac{1}{2}[A,B]}\, e^{iA}\, e^{iB}. \tag{3.3}$$

Analogously to (1.10) we define for this purpose

$$\hat{\boldsymbol{u}}_{\boldsymbol{m}} = U^{+} \begin{pmatrix} \boldsymbol{x}_{\boldsymbol{m}} \\ \boldsymbol{y}_{\boldsymbol{m}} \end{pmatrix};\ \begin{matrix} \{x_{\boldsymbol{m}i}, y_{\boldsymbol{n}_j}\} = 0, \\ \{x_{\boldsymbol{m}i}, \psi_{\boldsymbol{n}_j}\} = 0, \quad \{y_{\boldsymbol{m}i}\, \psi_{\boldsymbol{n}_j}\} = 0, \\ \{x_{\boldsymbol{m}i}, \psi^{+}_{\boldsymbol{n}_j}\} = 0, \quad \{y_{\boldsymbol{m}i}\, \psi^{+}_{\boldsymbol{n}_j}\} = 0. \end{matrix} \tag{3.4}$$

With that we find

$$C = (A+B) = \sum_{\boldsymbol{p}} \hat{\boldsymbol{u}}_{\boldsymbol{p}}^{\mathrm{T}} \cdot \hat{\boldsymbol{\psi}}_{\boldsymbol{p}} = \sum_{\boldsymbol{p}} (\boldsymbol{x}_{\boldsymbol{p}}^{\mathrm{T}}, \boldsymbol{y}_{\boldsymbol{p}}^{\mathrm{T}})\, U\, U^{\#} \begin{pmatrix} \boldsymbol{\psi}_{\boldsymbol{p}} \\ \boldsymbol{\psi}^{\#}_{\boldsymbol{p}} \end{pmatrix}$$
$$= \sum_{\boldsymbol{p}} (\boldsymbol{y}_{\boldsymbol{p}}^{\mathrm{T}} \cdot \boldsymbol{\psi}_{\boldsymbol{p}} + \boldsymbol{x}_{\boldsymbol{p}}^{\mathrm{T}} \cdot \boldsymbol{\psi}^{\#}_{\boldsymbol{p}}). \tag{3.5}$$

Now insertion of Λ^V and Λ^L makes the following decomposition possible:

$$A = : \sum_{\boldsymbol{p}} A_{\boldsymbol{p}} = \sum_{\boldsymbol{p}} (\boldsymbol{y}_{\boldsymbol{p}}^{\mathrm{T}} \Lambda_{\boldsymbol{p}}^V \boldsymbol{\psi}_{\boldsymbol{p}} + \boldsymbol{x}_{\boldsymbol{p}}^{\mathrm{T}} \Lambda_{\boldsymbol{p}}^L \boldsymbol{\psi}^{\#}_{\boldsymbol{p}}), \tag{3.6}$$

$$B = : \sum_{\boldsymbol{p}} B_{\boldsymbol{p}} = \sum_{\boldsymbol{p}} (\boldsymbol{y}_{\boldsymbol{p}}^{\mathrm{T}} \Lambda_{\boldsymbol{p}}^L \boldsymbol{\psi}_{\boldsymbol{p}} + \boldsymbol{x}_{\boldsymbol{p}}^{\mathrm{T}} \Lambda_{\boldsymbol{p}}^V \boldsymbol{\psi}^{\#}_{\boldsymbol{p}}). \tag{3.7}$$

$A_{\boldsymbol{p}}$ and $B_{\boldsymbol{p}}$ plays the role of new creation and destruction operators relative to the physical va-

cuum $|\mathfrak{o}\rangle$

$$B_p|\mathfrak{o}\rangle = 0, \quad \langle\mathfrak{o}|A_p = 0\,. \tag{3.8}$$

This "vacuum" may be a filled valence bandstate

$$|\mathfrak{o}\rangle = \prod_{p}\prod_{i=1}^{np}\psi_{pi}^{+}|0\rangle\,. \tag{3.9}$$

$|0\rangle$ is the bare vacuum state. (3.6) and (3.7) inserted into (3.3) yields (3.10)

$$\mathfrak{V} = \exp\{\tfrac{1}{2}\sum_{p}\hat{\boldsymbol{u}}_p^{\mathrm{T}}\hat{F}_p\hat{\boldsymbol{u}}_p\}\,\Phi\,. \tag{3.10}$$

Here is Φ a generating functional of the normal-ordered products. We define

$$\langle\alpha|\,\Phi\,|\beta\rangle = \sum_{n=0}^{\infty}\frac{i^n}{n!}\sum_{p_1\ldots p_n}\hat{\boldsymbol{u}}_{p_n}^{\mathrm{T}}\ldots\hat{\boldsymbol{u}}_{p_1}^{\mathrm{T}}\hat{\varphi}^n(\boldsymbol{p}_1\ldots\boldsymbol{p}_n) \tag{3.11}$$

where in analogy to (2.11) the "φ-functions" $\hat{\varphi}^n(\boldsymbol{p}_1\ldots\boldsymbol{p}_n)$ are antisymmetrical in the arguments $\boldsymbol{p}_i$. $\hat{F}_p$ may be evaluated by using

$$[A_p, B_p] = \boldsymbol{y}_p^{\mathrm{T}}(\Lambda_p^L - \Lambda_p^V)\boldsymbol{x}_p = \tfrac{1}{2}(\boldsymbol{x}_p^T, \boldsymbol{y}_p^T) \tag{3.12}$$

$$\cdot\begin{pmatrix} 0 & -(\Lambda_T^L - \Lambda_p^V) \\ (\Lambda_p^L - \Lambda_p^V) & 0 \end{pmatrix}\begin{pmatrix}\boldsymbol{x}_p \\ \boldsymbol{y}_p\end{pmatrix} = \hat{\boldsymbol{u}}_p^{\mathrm{T}}\hat{F}_p\hat{\boldsymbol{u}}_p\,.$$

with

$$\hat{F}_p = \tfrac{1}{2}U^{\mathrm{T}}\begin{pmatrix} 0 & -(\Lambda_p^L - \Lambda_p^V) \\ (\Lambda_p^L - \Lambda_p^V) & 0 \end{pmatrix}U$$

$$= \tfrac{1}{2}U^{+}\begin{pmatrix}(\Lambda_p^L - \Lambda_p^V) & 0 \\ 0 & -(\Lambda_p^L - \Lambda_p^V)\end{pmatrix}U\,. \tag{3.13}$$

We use the definitions

$$\hat{\Lambda}_p^{\mathrm{L}} = \tfrac{1}{2}U^{+}\begin{pmatrix}\Lambda_p^L & \\ & \Lambda_p^V\end{pmatrix}U; \quad \hat{\Lambda}_p^{\mathrm{V}} = \tfrac{1}{2}U^{+}\begin{pmatrix}\Lambda_p^V & \\ & \Lambda_p^L\end{pmatrix}U\,. \tag{3.14}$$

Now we obtain

$$\hat{F}_p = \hat{\Lambda}_p^{\mathrm{L}} - \hat{\Lambda}_p^{\mathrm{V}}\,. \tag{3.15}$$

The following relations hold

$$\hat{F}_p^{\mathrm{T}} = -\hat{F}_p\,; \quad (\hat{\Lambda}_p^L)^{\mathrm{T}} = \hat{\Lambda}_p^V; \quad (\hat{\Lambda}_p^V)^{\mathrm{T}} = \hat{\Lambda}_p^L\,. \tag{3.16}$$

§ 4. The φ-System

The transformation (3.10) yields a functional equation for the generating functional Φ. It will be enough to replace $\hat{\partial}_n$ by

$$\hat{\partial}_n \to \hat{\boldsymbol{D}}_n = \hat{\partial}_n + \hat{F}_n\hat{\boldsymbol{u}}_n\,. \tag{4.1}$$

Having taken into account the properties of anti-commutators and traces, we find a functional-equation

$$[\mathfrak{H}, \Phi]|0) = \mathfrak{F}(\hat{\boldsymbol{u}}, \hat{\boldsymbol{D}})\,\Phi\,|0) \tag{4.2}$$

which will be multiplied from the left and the right by $\langle\alpha|$ and $|\beta\rangle$. According to the method necessary to derive (2.12), we find the matrix system of φ-functions by comparison the powers of $\hat{\boldsymbol{u}}_P$. With the meaning of $\boldsymbol{m}'/i$; $1/j$; $1/j'$ explained in (2.12), the φ-system becomes

$$\omega\,\hat{\varphi}^k(\boldsymbol{n}_1\ldots\boldsymbol{n}_k) = \sum_{i=1}^{k}\sum_{\boldsymbol{n}\boldsymbol{n}'\boldsymbol{m}'}\hat{W}_{\boldsymbol{n}i\boldsymbol{n}\boldsymbol{n}'\boldsymbol{m}'}\hat{\varphi}^{k+2}(\boldsymbol{n}_1\ldots\boldsymbol{m}'/i\ldots\boldsymbol{n}_k\,\boldsymbol{n}'\,\boldsymbol{n})$$

$$-\sum_{i=1}^{k}\sum_{\boldsymbol{m}'}[\hat{H}_{\boldsymbol{n}_i\boldsymbol{m}'} + \hat{B}_{\boldsymbol{n}_i\boldsymbol{m}'} + \sum_{\boldsymbol{n}}(2\,\hat{W}_{\boldsymbol{n}_i\boldsymbol{n}\boldsymbol{m}'\boldsymbol{n}} - \hat{W}_{\boldsymbol{n}_i\boldsymbol{n}\boldsymbol{n}\boldsymbol{m}'})\hat{F}_{\boldsymbol{n}}]\hat{\varphi}^k(\boldsymbol{n}_1\ldots\boldsymbol{m}'/i\ldots\boldsymbol{n}_k)$$

$$-\sum_{ij=1}^{k}{}'\sum_{\boldsymbol{m}'\boldsymbol{n}'}[2\,\hat{F}_{\boldsymbol{n}_j}\hat{W}_{\boldsymbol{n}_i\boldsymbol{n}_j\boldsymbol{n}'\boldsymbol{m}'} + \hat{F}_{\boldsymbol{n}_i}\hat{W}_{\boldsymbol{n}'\boldsymbol{n}_i\boldsymbol{n}_j\boldsymbol{m}'}]\hat{\varphi}^k(\boldsymbol{n}_1\ldots\boldsymbol{m}'/i\ldots\boldsymbol{n}'/j\ldots\boldsymbol{n}_k)$$

$$+\sum_{ij}^{k}{}'\hat{F}_{\boldsymbol{n}_i}[\hat{H}_{\boldsymbol{n}_i\boldsymbol{n}_j} + \hat{B}_{\boldsymbol{n}_i\boldsymbol{n}_j} + \sum_{\boldsymbol{n}}(2\,\hat{W}_{\boldsymbol{n}_i\boldsymbol{n}\boldsymbol{n}_j\boldsymbol{n}} - \hat{W}_{\boldsymbol{n}_i\boldsymbol{n}\boldsymbol{n}\boldsymbol{n}_j})\hat{F}_{\boldsymbol{n}}](-1)^{P_{ij}}\hat{\varphi}^{k-2}(\boldsymbol{n}_1\ldots 1/i\ldots 1/j\ldots\boldsymbol{n}_k)$$

$$+\sum_{ijj'}^{k}{}'\sum_{\boldsymbol{m}'}[2\,\hat{F}_{\boldsymbol{n}_i}\hat{F}_{\boldsymbol{n}_j}\hat{W}_{\boldsymbol{n}_i\boldsymbol{n}_j\boldsymbol{n}_{j'}\boldsymbol{m}'} - \hat{F}_{\boldsymbol{n}_j}\hat{W}_{\boldsymbol{n}_i\boldsymbol{n}_j\boldsymbol{n}_{j'}\boldsymbol{m}'} + \tfrac{1}{4}\hat{W}_{\boldsymbol{n}_i\boldsymbol{n}_j\boldsymbol{n}_{j'}\boldsymbol{m}'}](-1)^{P_{jj'}}$$
$$\cdot\hat{\varphi}^{k-2}(\boldsymbol{n}_1\ldots\boldsymbol{m}'/i\ldots 1/j\ldots 1/j'\ldots\boldsymbol{n}_k)$$

$$-\sum_{ii'jj'=1}^{k}[\hat{F}_{\boldsymbol{n}_j}\hat{W}_{\boldsymbol{n}_i\boldsymbol{n}_j\boldsymbol{n}_{j'}\boldsymbol{n}_{i'}}\hat{F}_{\boldsymbol{n}_{j'}}\hat{F}_{\boldsymbol{n}_{i'}} - \tfrac{1}{4}\hat{W}_{\boldsymbol{n}_i\boldsymbol{n}_j\boldsymbol{n}_{j'}\boldsymbol{n}_{i'}}\hat{F}_{\boldsymbol{n}_{i'}}](-1)^{P_{jj'}}$$
$$\cdot\hat{\varphi}^{k-4}(\boldsymbol{n}_1\ldots 1/i\ldots 1/j\ldots 1/j'\ldots 1/i'\ldots\boldsymbol{n}_k)\,. \tag{4.3}$$

By means of restriction to a finite number of lattice points and a finite number of functions at these points, we find a maximum k for the order of the $\hat{\varphi}^k$'s. Pauli's law forbids at twofold action of the operators in the normal-ordered products in $\hat{\varphi}^k$. Therefore, (4.3) becomes a system of high, but finite dimension. This is of great importance for further investigations with regard to the problems of convergence of an infinite system.

We expect from the considerations of § 3, that a good approximation is obtained by truncating the system for small $N \geqq k$. However, it is not immediately obvious, how the different states are generated in the various steps of approximation. The discussion of the matrix elements in (4.3) and the calculations of the first approaches demonstrate, that we reach the expected states in the neighbourhood of the original state, which is fixed by a φ-transformation that contains a suitable choice of the projectors in $\hat{F}_p$.

§ 5. Interpretation of Matrixelements and the Lowest-Order Approximations

We obtain a first insight, if we cut the system (4.3) after $N=1$. So we are left with

$$\omega\,\hat{\varphi}(\boldsymbol{n}_i) + \sum_{\boldsymbol{m}} \hat{\mathfrak{H}}_{n_i m}\,\hat{\varphi}(\boldsymbol{m}) = 0 \tag{5.1}$$

where

$$\mathfrak{H}_{\boldsymbol{nm}} = \hat{H}_{\boldsymbol{nm}} + \hat{B}_{\boldsymbol{nm}} + \sum_{\boldsymbol{n}'} (2\,\hat{W}_{\boldsymbol{nn'mn'}} - \hat{W}_{\boldsymbol{nn'n'm}})\,\hat{F}_{\boldsymbol{n}'} \tag{5.2}$$

The use of (1.13) – (1.17) and $\hat{F}_{\boldsymbol{n}}$ from (3.13), and the insertion of $I = \Lambda_{\boldsymbol{n}}^L + \Lambda_{\boldsymbol{n}}^V$ between the matrixelements of $\hat{B}_{\boldsymbol{nm}}$ gives

$$\hat{\mathfrak{H}}_{\boldsymbol{nm}} = U^+ \begin{pmatrix} \mathfrak{H}_{\boldsymbol{nm}} & 0 \\ 0 & -\mathfrak{H}_{\boldsymbol{nm}}^{\mathrm{T}} \end{pmatrix} U \tag{5.3}$$

with

$$\mathfrak{H}_{\boldsymbol{nm}} = H_{\boldsymbol{nm}} + \iint \sum_{\boldsymbol{n}'} [A_{\boldsymbol{nm}}(\boldsymbol{r}_1)\,\mathrm{Tr}(A_{\boldsymbol{n'n'}}(\boldsymbol{r}_2)\,\Lambda_{\boldsymbol{n}'}^V) - A_{\boldsymbol{nn'}}(\boldsymbol{r}_1)\,\Lambda_{\boldsymbol{n}'}^V\,A_{\boldsymbol{n'm}}(\boldsymbol{r}_2)]\,\frac{e^2}{|\boldsymbol{r}_1 - \boldsymbol{r}_2|}\,\mathrm{d}\tau_1\,\mathrm{d}\tau_2 .$$

Since

$$H_{\boldsymbol{nm}}^{\mathrm{T}} = H_{\boldsymbol{mn}}^*; \quad A_{\boldsymbol{nm}}^{\mathrm{T}} = A_{\boldsymbol{mn}}^* \tag{5.4}$$

the second row of (5.3) consists of the negative complex conjugate matrix of the upper row. (5.3) can be interpreted, if we suppose that the functions $w_{\boldsymbol{mi}}(\boldsymbol{r})$ in the matrixelements are determined by a Hartree-Fock-approximation for an ideal crystal. If we use the Wannier functions

$$v_{\boldsymbol{mi}}(\boldsymbol{r} - \boldsymbol{R}_m) = \frac{1}{\sqrt{N}} \sum_{\boldsymbol{k}} b_{\boldsymbol{ki}}(\boldsymbol{r})\,\mathrm{e}^{-i\,\boldsymbol{k}\cdot\boldsymbol{m}} \tag{5.4 a}$$

where

$$b_{\boldsymbol{ki}}(\boldsymbol{r}) = u_{\boldsymbol{ki}}(\boldsymbol{r})\,e^{i\,\boldsymbol{k}\cdot\boldsymbol{r}}; \quad u_{\boldsymbol{ki}}(\boldsymbol{r} + \boldsymbol{R}_n) = u_{\boldsymbol{ki}}(\boldsymbol{r}) \tag{5.4 b}$$

are Bloch-functions, we get with the aid of the translations $\boldsymbol{r}_s = \boldsymbol{r}_s + R_{\boldsymbol{n}}$ $(s = 1, 2)$ in detail

$$\begin{aligned} \mathfrak{H}_{\substack{\boldsymbol{nm}\\ k\,l}}^{(J)} &= \frac{1}{N} \int \mathrm{d}\tau' \sum_{\boldsymbol{k}k} b_{\boldsymbol{k}k}^*(\boldsymbol{r}') \\ &\cdot \left[-\frac{\hbar^2}{2\,m}\,\Delta + \sum_{\boldsymbol{h}a} \frac{e\,e_a}{|\boldsymbol{r}' - \boldsymbol{R}_{\boldsymbol{h}a}|} \right] b_{\boldsymbol{k}'l}(\boldsymbol{r}')\,e^{i\,\boldsymbol{k}'\cdot(\boldsymbol{n}-\boldsymbol{m})} \\ &+ \frac{1}{N} \iint \mathrm{d}\tau_1'\,\mathrm{d}\tau_2' \sum_{\boldsymbol{k}\boldsymbol{k}'l} \sum_{i \in V} [b_{\boldsymbol{k}k}^*(\boldsymbol{r}_1')\,b_{\boldsymbol{k}'l}(\boldsymbol{r}_1') \\ &\cdot b_{li}^*(\boldsymbol{r}_2')\,b_{li}(\boldsymbol{r}_2') - b_{\boldsymbol{k}k}^*(\boldsymbol{r}_1')\,b_{li}(\boldsymbol{r}_1')\,b_{li}^*(\boldsymbol{r}_2')\,b_{\boldsymbol{k}'l}(\boldsymbol{r}_2')] \\ &\cdot \frac{e^{i\,\boldsymbol{k}'\cdot(\boldsymbol{n}-\boldsymbol{m})}}{|\boldsymbol{r}_1' - \boldsymbol{r}_2'|} = \frac{1}{N} \sum_{\boldsymbol{k}\boldsymbol{k}'} \varepsilon_{kl}(\boldsymbol{k}, \boldsymbol{k}')\,e^{i\,\boldsymbol{k}'\cdot(\boldsymbol{n}-\boldsymbol{m})} . \end{aligned} \tag{5.5}$$

Here the summation over $\boldsymbol{l}$, i include Bloch-functions of the valence bands only, provided that the $\Lambda_{\boldsymbol{n}}^V$ are determined in a manner which covers the manifold of valence-band-functions. If $b_{\boldsymbol{k}k}$ and $b_{\boldsymbol{k},l}$ are themselves functions of the valence-bands, they drop out in the summation over $\boldsymbol{l}$, i. Variation of (5.5) with respect to $b_{\boldsymbol{k}}^*$ subjected to the condition

$$\int b_{\boldsymbol{k}k}^*(\boldsymbol{r})\,b_{\boldsymbol{k}l}(\boldsymbol{r})\,\mathrm{d}\tau = \delta_{k,k'}\,\delta_{k,l} \tag{5.6}$$

yields the integro-differential equations of the Hartree-Fock method. On the other hand, if the $b_{\boldsymbol{k}k}$'s are already determined by such a method, we have instead of (5.5) the diagonalized form

$$\begin{aligned} \mathfrak{H}_{\substack{\boldsymbol{nm}\\ k\,l}}^{(J)} &= \frac{1}{N} \sum_{\boldsymbol{k}\boldsymbol{k}'} \delta_{k,k'}\,\delta_{k,l}\,\varepsilon_{kl}(\boldsymbol{k}, \boldsymbol{k}')\;e^{i\,\boldsymbol{k}\cdot(\boldsymbol{n}-\boldsymbol{m})} \\ &= \frac{1}{N} \sum_{\boldsymbol{k}} \varepsilon_k(\boldsymbol{k})\,e^{i\,\boldsymbol{k}\cdot(\boldsymbol{n}-\boldsymbol{m})} \end{aligned} \tag{5.7}$$

or in matrixform, with diagonalmatrices $\mathcal{E}(\boldsymbol{k}) = \mathcal{E}(\boldsymbol{k})^{\mathrm{T}}$

$$\hat{\mathfrak{H}}_{\boldsymbol{nm}}^{(J)} = \frac{1}{N} \sum_{\boldsymbol{k}} e^{i\,\boldsymbol{k}\cdot(\boldsymbol{n}-\boldsymbol{m})}\,U^+ \begin{pmatrix} \mathcal{E}(\boldsymbol{k}) & 0 \\ 0 & -\mathcal{E}(\boldsymbol{k}) \end{pmatrix} U . \tag{5.8}$$

$\mathcal{E}_k(\boldsymbol{k})$ is the one-particle energy of an electron in the periodic potential of all valence-band electrons and all nuclei of the crystal. Therefore, it is the energy of an additional electron, provided k belongs to a function in a conduction band, or it is the negative of a hole, if $k \in V$. With (5.8) the eigenwertproblem (5.1) is immediately soluble. We define, in analogy to (1.10)

$$\hat{\varphi}(\boldsymbol{m}) = U^+ \begin{pmatrix} \varphi(\boldsymbol{m}) \\ \varphi^{\#}(\boldsymbol{m}) \end{pmatrix} = \frac{1}{\sqrt{N}} \sum_{\boldsymbol{k}} U^+ \begin{pmatrix} \varphi_{\boldsymbol{k}} \\ \varphi_{\boldsymbol{k}}^{\#} \end{pmatrix} e^{i\,\boldsymbol{k}\cdot\boldsymbol{m}} . \tag{5.9}$$

After insertion of (5.9) into (5.1), multiplication $1/\sqrt{N}\; e^{-i\,\boldsymbol{k}\cdot\boldsymbol{m}}\,U$ from the left and summation over $\boldsymbol{m}'=\boldsymbol{n}-\boldsymbol{m}$, the system decouples in two parts

$$(\omega I+\mathcal{E}(\boldsymbol{k}))\varphi_{\boldsymbol{k}}=0\,, \qquad (5.10\,\text{a})$$

$$\varphi_{\boldsymbol{k}}^{+}(\omega I-\mathcal{E}(\boldsymbol{k}))=0\,. \qquad (5.10\,\text{b})$$

Besides the sign of $\mathcal{E}(\boldsymbol{k})$, (5.10 b) is identical to (5.10 a). This fact will be revealed, when we calculate energy differences, where in the first case (10 a) $|\alpha\rangle$ means the starting state, here the Hartree-Fock-approximation of the groundstate, and $|\beta\rangle$ the additional electron state. In the other case (10 b), the roles of the states $|\alpha\rangle$ and $|\beta\rangle$ are interchanged. We conclude:

1. The lowest approximation yields energy differences between a starting state with $n=\sum_{\boldsymbol{p}} n_{\boldsymbol{p}}$ electrons, represented by the entirety of the projection operators $\Lambda_{\boldsymbol{p}}^{V}$, and the $(n+1)$-, respectively $(n-1)$. electron states in the neighbourhood of the first.

2. Every state with energy differences $\omega_{\alpha\beta}$ is accompanied by a state with $-\omega_{\alpha\beta}$. Theorem 2 is a general statement, theorem 1 can be generalized to higher states, calculated by higher-order approximations. In which sequence such higher states appear, is not yet clear, however, the treatment of an exciton state in this paper gives some insight.

Now we look at the fourth expression at the right-hand side of (4.3). With (5.2) and the assumption (5.8), which means that we use the Hartree-Fock functions, we obtain

$$\sum_{ij=1}^{k}{}' \hat{F}_{\boldsymbol{n}_i}\,\hat{\mathfrak{H}}_{\boldsymbol{n}_i\boldsymbol{n}_j}^{(J)}\,(-1)^{P_{ij}}\,\hat{\varphi}^{k-2}\,(\boldsymbol{n}_1\ldots 1/i\ldots 1/j\ldots\boldsymbol{n}_k)=\tfrac{1}{2}\sum_{ij}{}'\,(\hat{F}_{\boldsymbol{n}_i}\,\hat{\mathfrak{H}}_{\boldsymbol{n}_i\boldsymbol{n}_j}^{(J)}-\hat{\mathfrak{H}}_{\boldsymbol{n}_i\boldsymbol{n}_j}^{(J)}\,\hat{F}_{\boldsymbol{n}_j})\,(-1)^{P_{ij}}$$

$$\cdot\,\hat{\varphi}^{k-2}\,(\boldsymbol{n}_1\ldots 1/i\ldots 1/j\ldots\boldsymbol{n}_k)$$

$$=-\tfrac{1}{2}\sum_{ij}{}'\,U^{+}\begin{pmatrix}P_{\boldsymbol{n}_i\boldsymbol{n}_j} & 0\\ 0 & -P_{\boldsymbol{n}_i\boldsymbol{n}_j}^{\mathrm{T}}\end{pmatrix}U\,e^{i\,\boldsymbol{k}\cdot(\boldsymbol{n}_i-\boldsymbol{n}_j)}\,(-1)^{P_{ij}}\hat{\varphi}^{k-2}\,(\boldsymbol{n}_1\ldots 1/i\ldots 1/j\ldots n_k),$$

$$P_{\boldsymbol{n}_i\boldsymbol{n}_j}=(\Lambda_{\boldsymbol{n}_i}^{L}-\Lambda_{\boldsymbol{n}_i}^{V})\,\mathcal{E}(\boldsymbol{k})-\mathcal{E}(\boldsymbol{k})\,(\Lambda_{\boldsymbol{n}_j}^{L}-\Lambda_{\boldsymbol{n}_j}^{V}). \qquad (5.11)$$

In case the $\Lambda_{\boldsymbol{n}}^{L}$ and $\Lambda_{\boldsymbol{n}}^{V}$ are all identical for every $\boldsymbol{n}$, as in (5.5) where we transformed to Bloch functions, (5.11) vanishes.

§ 6. The Resolvents of the Ideal Crystal

For the calculation of boundstates it is useful, and generally necessary, to compute the inversion of the one-electron part in (4.3). If the crystal is not largely disturbed, it is enough to invert the part, which belongs to an ideal crystal. For this purpose we write (4.3) in the form

$$\omega\,\hat{\varphi}^{k}(\boldsymbol{n}_1\ldots\boldsymbol{n}_k)+\sum_{i=1}^{k}\sum_{\boldsymbol{m}}\hat{\mathfrak{H}}_{\boldsymbol{n}_i\boldsymbol{m}}^{(J)}\,\hat{\varphi}^{k}(\boldsymbol{n}_1\ldots\boldsymbol{m}/i\ldots\boldsymbol{n}_{\mathrm{k}})=\hat{R}(\boldsymbol{n}_1\ldots\boldsymbol{n}_k) \qquad (6.1)$$

where $\hat{\mathfrak{H}}_{\boldsymbol{n}\boldsymbol{m}}^{(J)}$ is the one-electron energy of an ideal crystal defined by (5.2) and (5.8). On the right-hand side stands

$$\hat{R}(\boldsymbol{n}_1\ldots\boldsymbol{n}_k)=-\sum_{i=1}^{k}\sum_{\boldsymbol{m}}(\hat{\mathfrak{H}}_{\boldsymbol{n}_i\boldsymbol{m}}-\hat{\mathfrak{H}}_{\boldsymbol{n}_i\boldsymbol{m}}^{(J)})\,\hat{\varphi}^{k}(\boldsymbol{n}_1\ldots\boldsymbol{m}/i\ldots\boldsymbol{n}_k)+\hat{R}^{0}(\boldsymbol{n}_1\ldots\boldsymbol{n}_k) \qquad (6.2)$$

meaning the difference between the one-electron parts of disturbed and ideal crystals, plus $\hat{R}^{0}$, which is the total of the remaining terms on the right-hand side of (4.3). Inverting the left-hand side of (6.1)

$$\hat{\varphi}^{k}(\boldsymbol{n}_1\ldots\boldsymbol{n}_k)=\sum_{\boldsymbol{n}_1'\ldots\boldsymbol{n}_k'}\hat{G}\,(\boldsymbol{n}_1-\boldsymbol{n}_1',\ldots,\boldsymbol{n}_k-\boldsymbol{n}_k'\,|\,\omega)\,\hat{R}(\boldsymbol{n}_1'\ldots\boldsymbol{n}_k') \qquad (6.3)$$

we are faced with the problem to calculate the resolvents $\hat{G}(\boldsymbol{n}_1-\boldsymbol{n}_1',\ \ldots,\ \boldsymbol{n}_k-\boldsymbol{n}_k'\,|\,\omega)$. For this reason we define a new kind of projection operators I_l, which projects out exactly the l-th one-electron energy $\varepsilon_l(\boldsymbol{k})$ from the energy matrix $\mathcal{E}(\boldsymbol{k})$

$$I_l\,\mathcal{E}(\boldsymbol{k})=\varepsilon_l(\boldsymbol{k})\,;\qquad \sum_{l=1}^{m+n}I_l=I$$

where I = identity matrix in $m+n$ dimensional space of energy bands.

We extend the definition to

$$\hat{I}_l^{+}=U^{+}\begin{pmatrix}I_l & \\ & 0\end{pmatrix}U;\qquad \hat{I}_l^{-}=U^{+}\begin{pmatrix}0 & \\ & I_l\end{pmatrix}U; \qquad (6.5)$$

$$\hat{I} = \hat{I}^{+} + \hat{I}^{-}; \qquad \hat{I}^{+} = \sum_{l} \hat{I}_{l}^{+}; \qquad \hat{I}^{-} = \sum_{l} I_{l}^{-}. \tag{6.6}$$

Thereafter we change to Fourier representation

$$\varphi^{k}(\boldsymbol{n}_1 \ldots \boldsymbol{n}_k) = \frac{1}{\sqrt{N^k}} \varphi(\boldsymbol{k}_1 \ldots \boldsymbol{k}_k)\ e^{i(\boldsymbol{k}_1 \cdot \boldsymbol{n}_1 + \ldots + \boldsymbol{k}_k \cdot \boldsymbol{n}_k)} \tag{6.7}$$

and then we can write (6.1) in the following form

$$\sum_{i=1}^{k} \sum_{\boldsymbol{k}_1 \ldots \boldsymbol{k}_k} \left(\hat{I}_{(1)} \times \hat{I}_{(2)} \times \ldots \times U_{(i)}^{+} \begin{pmatrix} \omega + \mathcal{E}(\boldsymbol{k}_i) & 0 \\ 0 & \omega - \mathcal{E}(\boldsymbol{k}_i) \end{pmatrix} U_{(i)} \times \ldots \times \hat{I}_{(k)} \right)$$
$$\cdot \frac{1}{\sqrt{N^k}}\, e^{i(\boldsymbol{k}_1 \cdot \boldsymbol{n}_1 + \ldots + \boldsymbol{k}_k \cdot \boldsymbol{n}_k)}\, \hat{\varphi}(\boldsymbol{k}_1 \ldots \boldsymbol{k}_k) = \hat{R}(\boldsymbol{n}_1 \ldots \boldsymbol{n}_k). \tag{6.8}$$

The indices in the brackets indicate the position. Multiplication from the right with the projection operator

$$\frac{1}{\sqrt{N^k}} \exp\{-i(\boldsymbol{k}_1' \cdot \boldsymbol{n}_1 + \ldots + \boldsymbol{k}_k' \cdot \boldsymbol{n}_k)\}\, \hat{P}^{\pm\pm\cdots\pm}_{l_1 l_2 \ldots l_k} := \frac{1}{\sqrt{N^k}} \hat{I}^{\pm}_{l_1} \times \hat{I}^{\pm}_{l_2} \times \ldots \times \hat{I}^{\pm}_{l_k} \exp\{-i(\boldsymbol{k}_1' \cdot \boldsymbol{n}_1 + \ldots + \boldsymbol{k}_k' \cdot \boldsymbol{n}_k)\} \tag{6.9}$$

yields, after summation over $\boldsymbol{n}_1, \boldsymbol{n}_2, \ldots, \boldsymbol{n}_k$

$$[\omega + (\pm \varepsilon_{l_1}(\boldsymbol{k}_1) + (\pm \varepsilon_{l_2}(\boldsymbol{k}_2) + \ldots + (\pm \varepsilon_{l}(\boldsymbol{k}_k))] \hat{P}^{\pm\pm\cdots\pm}_{l_1 l_2 \ldots l_k}\, \hat{\varphi}(\boldsymbol{k}_1' \ldots \boldsymbol{k}_k')$$
$$= \sum_{\boldsymbol{n}_1 \ldots \boldsymbol{n}_k} \hat{P}^{\pm\pm\cdots\pm}_{l_1 l_2 \ldots l_k} \frac{1}{\sqrt{N^k}} \exp\{-i(\boldsymbol{k}_1' \boldsymbol{n}_1 + \ldots + \boldsymbol{k}_k \cdot \boldsymbol{n}_k)\} \hat{R}(\boldsymbol{n}_1 \ldots \boldsymbol{n}_k). \tag{6.10}$$

Now we are able to divide the bracket on the left and then go back to the representation in configuration space. With $\sum^{k}_{\pm}$ as a symbol for summation over the 2^k terms $I^{\pm}_{(1)} \times I^{\pm}_{(2)} \times \ldots \times I^{\pm}_{(k)}$ we get

$$\sum_{l_1 \ldots l_k} \sum^{k}_{\pm} \hat{P}^{\pm\pm\cdots\pm}_{l_1 l_2 \ldots l_k} = \hat{I}_{(1)} \times \hat{I}_{(2)} \times \ldots \times \hat{I}_{(k)} \tag{6.11}$$

consequently

$$\hat{G}(\boldsymbol{n}_1 - \boldsymbol{n}_1', \ldots, \boldsymbol{n}_k - \boldsymbol{n}_k' \,|\, \omega) = \frac{1}{N^k} \sum_{\substack{\boldsymbol{k}_1 \ldots \boldsymbol{k}_k \\ l_1 \ldots l_k}} \sum^{k}_{\pm} \frac{\hat{P}^{\pm\pm\cdots\pm}_{l_1 l_2 \ldots l_k} \exp\{i\,(\boldsymbol{k}_1 \cdot (\boldsymbol{n}_1 - \boldsymbol{n}_1') + \ldots \boldsymbol{k}_k (\boldsymbol{n}_k - \boldsymbol{n}_k'))}{\omega + \sum_{i=1}^{k} (\pm \varepsilon_{l_i}(\boldsymbol{k}_i))}. \tag{6.12}$$

§ 7. Two-Body States

Two-body problems are covered by truncating the system (4.3) at N = 2. Since $\hat{\varphi}^0 = \langle \alpha \,|\, \beta \rangle$ does not exist for $\omega \neq 0$, in which case $|\alpha\rangle \neq |\beta\rangle$ and therefore $\langle \alpha \,|\, \beta \rangle = 0$, the only equation for even k is

$$\hat{\varphi}^2(\boldsymbol{n}_1 \boldsymbol{n}_2) = \sum \hat{G}(\boldsymbol{n}_1 - \boldsymbol{n}_1', \boldsymbol{n}_2 - \boldsymbol{n}_2' \,|\, \omega) = \hat{R}(\boldsymbol{n}_1' \boldsymbol{n}_2') \tag{7.1}$$

with (6.2) and

$$\hat{R}^0(\boldsymbol{n}_1 \boldsymbol{n}_2) = -\sum_{\boldsymbol{m}'\boldsymbol{n}'} (2\, \hat{F}_{\boldsymbol{n}_2} \hat{W}_{\boldsymbol{n}_1 \boldsymbol{n}_2 \boldsymbol{n}' \boldsymbol{m}'} + 2\, \hat{F}_{\boldsymbol{n}_1} \hat{W}_{\boldsymbol{n}_2 \boldsymbol{n}_1 \boldsymbol{n}' \boldsymbol{m}'} + \hat{F}_{\boldsymbol{n}_1} \hat{W}_{\boldsymbol{n}' \boldsymbol{n}_1 \boldsymbol{n}_2 \boldsymbol{m}'} - \hat{F}_{\boldsymbol{n}_2} \hat{W}_{\boldsymbol{n}' \boldsymbol{n}_2 \boldsymbol{n}_1 \boldsymbol{m}'}) \hat{\varphi}^2(\boldsymbol{m}' \boldsymbol{n}')$$
$$= -2 \iint \mathrm{d}\tau_1\, \mathrm{d}\tau_2 \sum_{\boldsymbol{m}'\boldsymbol{n}'} \Bigg\{ \Bigg[2\, \hat{A}^{L}_{\boldsymbol{n}_1}\, \hat{A}_{\boldsymbol{n}_1 \boldsymbol{m}'}(\boldsymbol{r}_1) \frac{e_2}{|\boldsymbol{r}_1 - \boldsymbol{r}_2|}\, \hat{A}^{L}_{\boldsymbol{n}_2} \hat{A}_{\boldsymbol{n}_2 \boldsymbol{n}'}(\boldsymbol{r}_2) - 2\, \hat{A}^{V}_{\boldsymbol{n}_1} \hat{A}_{\boldsymbol{n}_1 \boldsymbol{m}'} \frac{e_2}{|\boldsymbol{r}_1 - \boldsymbol{r}_2|}\, \hat{A}^{V}_{\boldsymbol{n}_2} \hat{A}_{\boldsymbol{n}_2 \boldsymbol{n}'}(\boldsymbol{r}_2) \Bigg]$$
$$+ \hat{\varphi}(\boldsymbol{m}' \boldsymbol{n}') \left[\hat{A}^{L}_{\boldsymbol{n}_1}\, \hat{A}_{\boldsymbol{n}_1 \boldsymbol{n}_2}(\boldsymbol{r}_1) \hat{A}^{V}_{\boldsymbol{n}_2} - \hat{A}^{V}_{\boldsymbol{n}_1}\, \hat{A}_{\boldsymbol{n}_1 \boldsymbol{n}_2}(\boldsymbol{r}_1) \hat{A}^{L} \right] \frac{e_2}{|\boldsymbol{r}_1 - \boldsymbol{r}_2|} \sum_{\boldsymbol{m}'\boldsymbol{n}'} \mathrm{Tr}\, (\hat{A}_{\boldsymbol{n}_1 \boldsymbol{m}'}(\boldsymbol{r}_2)\, \hat{\varphi}_2(\boldsymbol{m}' \boldsymbol{n}')) \Bigg\}. \tag{7.2}$$

In order to arrive soon at some physical statements, we introduce a simplified crystal model, which contains only one conduction band with band energy $\varepsilon_0(\boldsymbol{k}) \equiv \varepsilon_L(\boldsymbol{k})$ and three valence bands with energies $\varepsilon_1(\boldsymbol{k}) = \varepsilon_2(\boldsymbol{k}) = \varepsilon_3(\boldsymbol{k}) \equiv \varepsilon_V(\boldsymbol{k})$. The appropriate Wannier functions may be highly localized, so there is only little overlap between functions at various lattice points. The idea of this concept is, that we have a crystal with closed shells of ions in form of p-functions and possible excited s-func-

tions at the same lattice point. An example may be KCl or NaCl. In our simplified model we will not distinguish between functions in the shells fo Cl- and K^+-ions.

With those restrictions we get

$$\Lambda_{\boldsymbol{n}}^L = I_0 \quad \Lambda_{\boldsymbol{n}}^V = \sum_{l=1}^{3} I_l \quad \text{for all } \boldsymbol{n} \tag{7.3}$$

and approximately

$$\hat{A}_{\boldsymbol{nm}}\ (\boldsymbol{r}) \approx \delta_{\boldsymbol{nm}}\ \hat{A}_{\boldsymbol{nn}}\ (\boldsymbol{r}) =: \delta_{\boldsymbol{nm}}\ \hat{A}(\boldsymbol{r}). \tag{7.4}$$

In the case of an ideal crystal, (7.2) is invariant relative to translations $\boldsymbol{n} = \boldsymbol{n}_1 - \boldsymbol{n}_2$ and $\hat{R}$ becomes equal to $\hat{R}^0$. We separate the centre-of-mass momentum $\boldsymbol{K}$ by the ansatz

$$\hat{\varphi}\ (\boldsymbol{n}_1\, \boldsymbol{n}_2) = 1/\sqrt{N} \sum_{\boldsymbol{k}} \varphi_{\boldsymbol{k}}\ (\boldsymbol{n})\, e^{i\cdot \boldsymbol{K}\cdot \boldsymbol{N}}, \tag{7.5}$$

$$\boldsymbol{N} = \tfrac{1}{2}(\boldsymbol{n}_1 + \boldsymbol{n}_2),\ \boldsymbol{n} = \boldsymbol{n}_1 - \boldsymbol{n}_2,$$
$$\boldsymbol{K} = \boldsymbol{k}_1 + \boldsymbol{k}_2,\ \boldsymbol{k} = \tfrac{1}{2}(\boldsymbol{k}_1 - \boldsymbol{k}_2).$$

and obtain from (7.2)

$$\hat{R}(\boldsymbol{n}_1\, \boldsymbol{n}_2) = \frac{1}{\sqrt{N}} \sum_{\boldsymbol{k}} \hat{R}_{\boldsymbol{K}}\ (\boldsymbol{n})\, e^{i\boldsymbol{K}\cdot \boldsymbol{N}} \tag{7.6}$$

with

$$\hat{R}_{\boldsymbol{K}}(\boldsymbol{n}) = -2 \iint \mathrm{d}\tau_1\, \mathrm{d}\tau_2$$
$$\Big\{\Big[2\, \hat{\Lambda}^L\, \hat{A}(\boldsymbol{r}_1)\, \frac{e^2}{|\boldsymbol{r}_1 - \boldsymbol{r}_2 + \boldsymbol{R}_{\boldsymbol{n}_1} - \boldsymbol{R}_{\boldsymbol{n}_2}|}\, \hat{\Lambda}^L\, \hat{A}(\boldsymbol{r}_2)$$
$$- 2\, \hat{\Lambda}^V\, \hat{A}(\boldsymbol{r}_1)\, \frac{e^2}{|\boldsymbol{r}_1 - \boldsymbol{r}_2 + \boldsymbol{R}_{\boldsymbol{n}_1} - \boldsymbol{R}_{\boldsymbol{n}_2}|}\, \hat{\Lambda}^V\, \hat{A}(\boldsymbol{r}_2)\Big]\, \hat{\varphi}_{\boldsymbol{K}}\ (\boldsymbol{n}) \tag{7.7}$$
$$+ \delta_{\boldsymbol{n}_1 \boldsymbol{n}_2} \sum_{\boldsymbol{q}} [\hat{\Lambda}^L\, \hat{A}(\boldsymbol{r}_1)\, \hat{\Lambda}^V$$
$$- \hat{\Lambda}^V\, \hat{A}(\boldsymbol{r}_1)\, \hat{\Lambda}^L]\, \frac{e^2\, e^{-i\boldsymbol{K}\cdot \boldsymbol{q}}}{|\boldsymbol{r}_1 - \boldsymbol{r}_2 + \boldsymbol{R}_{\boldsymbol{q}}|}\, \mathrm{Tr}\,(\hat{A}(\boldsymbol{r}_2)\, \hat{\varphi}_{\boldsymbol{K}}\,(0))\Big\}.$$

For the multiplication of $\hat{G}(\boldsymbol{n}_1 - \boldsymbol{n}_1',\ \boldsymbol{n}_2 - \boldsymbol{n}_2'/\omega)$ with $R_{\boldsymbol{K}}$, we note the following relations

$$\sum_l \hat{I}_l^+\, \hat{\Lambda}^L = \tfrac{1}{2}\hat{I}_0^+;\ \sum_l \hat{I}_l^-\, \hat{\Lambda}^L = \tfrac{1}{2}\sum_{l=1}^{3} \hat{I}_l^-; \tag{7.8}$$
$$\sum_l \hat{I}_l^+\, \hat{\Lambda}^V = \tfrac{1}{2}\sum_{l=1}^{3} I_l^+;$$
$$\sum_l \hat{I}_l^-\, \hat{\Lambda}^V = \tfrac{1}{2}\hat{I}_0^-; \qquad (\hat{I}_l^{\pm})^T = \hat{I}_l^{\mp},$$

and (3.16). Therefore, we get from (7.1)

$$\hat{\varphi}_{\boldsymbol{K}}(\boldsymbol{n}) = \sum_{\boldsymbol{k}} (K_{\boldsymbol{k}}^{++} + K_{\boldsymbol{k}}^{+-} + K_{\boldsymbol{k}}^{-+} + K_{\boldsymbol{k}}^{--})\, (C_{\boldsymbol{nk}} + D_{\boldsymbol{nk}}) \tag{7.9}$$

where

$$K_{\boldsymbol{k}}^{++} = \frac{\hat{I}_0^+ \times \hat{I}_0^+}{\omega + \varepsilon_L(1) + \varepsilon_L(2)} - \frac{\sum_{l_1=1}^{3} \hat{I}_{l_1}^+ \times \sum_{l_2=1}^{3} \hat{I}_{l_2}^+}{\omega + \varepsilon_V(1) - \varepsilon_V(2)},$$

$$K_{\boldsymbol{k}}^{-+} = \frac{\sum_{l_1=1}^{3} \hat{I}_{l_1}^- \times \hat{I}_0^+}{\omega - \varepsilon_V(1) + \varepsilon_L(2)} - \frac{\hat{I}_0^- \times \sum \hat{I}_{l_2}^+}{\omega - \varepsilon_L(1) + \varepsilon_V(2)},$$

$$K_{\boldsymbol{k}}^{+-} = \frac{\hat{I}_0^+ \times \sum_{l_2=1}^{3} \hat{I}_{l_2}^-}{\omega + \varepsilon_L(1) - \varepsilon_V(2)} - \frac{\sum_{l_1=1}^{3} \hat{I}_{l_1}^+ \times \hat{I}_0^-}{\omega + \varepsilon_V(1) - \varepsilon_L(2)},$$

$$K_{\boldsymbol{k}}^{--} = \frac{\sum_{l_1=1}^{3} \hat{I}_{l_1}^- \times \sum_{l_2=1}^{3} \hat{I}_{l_2}^-}{\omega - \varepsilon_V(1) - \varepsilon_V(2)} - \frac{\hat{I}_0^- \times \hat{I}_0^-}{\omega - \varepsilon_L(1) - \varepsilon_L(2)},$$

$$\varepsilon(1) \equiv \varepsilon(\tfrac{1}{2}\boldsymbol{K} + \boldsymbol{k}), \quad \varepsilon(2) \equiv \varepsilon(\tfrac{1}{2}\boldsymbol{K} - \boldsymbol{k}), \tag{7.10}$$

$$(C_{\boldsymbol{nk}})_{kl} = -\sum_{\boldsymbol{n}'} \sum_{ij} \frac{e^{i\,\boldsymbol{k}\,\cdot\,(\boldsymbol{n}-\boldsymbol{n}')}}{N} \iint (\hat{A}(\boldsymbol{r}_1))_{ki}$$
$$\cdot \frac{e^2}{|\boldsymbol{r}_1 - \boldsymbol{r}_2 + \boldsymbol{R}_{\boldsymbol{n}'}|}\, (\hat{A}(\boldsymbol{r}_2))_{lj}\, \hat{\varphi}_{\boldsymbol{K}\,ij}(\boldsymbol{n}')\cdot \mathrm{d}\tau_1\, \mathrm{d}\tau_2, \tag{7.11}$$

$$(D_{\boldsymbol{nk}})_{kl} = -\sum_{\boldsymbol{n}'} \delta_{n',0}\, \frac{e^{i\boldsymbol{k}\cdot(\boldsymbol{n}-\boldsymbol{n}')}}{N} \iint (\hat{A}(\boldsymbol{r}_1))_{kl}$$
$$\cdot \sum_{\boldsymbol{q}} \frac{e^2\, e^{-i\,\boldsymbol{K}\,\cdot\,\boldsymbol{q}}}{|\boldsymbol{r}_1 - \boldsymbol{r}_2 + \boldsymbol{R}_{\boldsymbol{q}}|} \sum_{ij} (\hat{A}(\boldsymbol{r}_2))_{ji}\, \hat{\varphi}_{\boldsymbol{K}\,ij}(0)\, \mathrm{d}\tau_1\, \mathrm{d}\tau_2. \tag{7.12}$$

The system (7.9) breaks up into four parts. This can be demonstrated by application of the projections $\hat{I}^{\pm} \times \hat{I}^{\pm}$ and the use of

$$\hat{I}^+ \hat{A} \hat{I}^+ = \hat{U}^+ \begin{pmatrix} A & 0 \\ 0 & 0 \end{pmatrix} U; \quad \hat{I}^- \hat{A} \hat{I}^- = \hat{U}^+ \begin{pmatrix} 0 & 0 \\ 0 & -A^{\mathrm{T}} \end{pmatrix} U, \tag{7.13}$$

$$\hat{I}^+ \hat{A} \hat{I}^- = \hat{I}^- \hat{A} \hat{I}^+ = 0. \tag{7.14}$$

We define

$$\hat{\varphi}^{\pm\pm} := (\hat{I}^{\pm} \times \hat{I}^{\pm})\, \hat{\varphi} \tag{7.15}$$

and get at first

$$\hat{\varphi}_{\boldsymbol{K}}^{++}\ (\boldsymbol{n}) = \sum K_{\boldsymbol{k}}^{++}\, C_{\boldsymbol{nk}} \quad \text{where} \quad C_{\boldsymbol{nk}} = C_{\boldsymbol{nk}}\,(\hat{\varphi}^{++}), \tag{7.16}$$

and secondly

$$\hat{\varphi}_{\boldsymbol{K}}^{--}\ (\boldsymbol{n}) = \sum K_{\boldsymbol{k}}^{--}\, C_{\boldsymbol{nk}} \quad \text{where} \quad C_{\boldsymbol{nk}} = C_{\boldsymbol{nk}}\,(\hat{\varphi}^{--}), \tag{7.17}$$

since with (7.14)

$$K_{\boldsymbol{k}}^{++}\, D_{\boldsymbol{nk}} = K_{\boldsymbol{k}}^{--}\, D_{\boldsymbol{nk}} = 0. \tag{7.18}$$

We want to prove that (7.16) changes to (7.17) by transposition and replacing ω by $-\omega$. That means, both systems contain the same solutions with the only difference, that the role of $|\alpha\rangle$ and $|\beta\rangle$ is exchanged. An exact analysis, analogously to § 8, shows that (7.16) and (7.17) describe the interaction of two additional electrons as well as the interaction of two defect electrons. Both are weakly coupled.

Another situation arises from the remaining two systems

$$\hat{\varphi}^{+-}_{\boldsymbol{K}}(\boldsymbol{n}) = \sum_{\boldsymbol{k}} K^{+-}_{\boldsymbol{k}} \left[C_{\boldsymbol{nk}}(\hat{\varphi}^{+-}) + D^{+-}_{\boldsymbol{nk}}(\hat{\varphi}^{+-}, \hat{\varphi}^{-+})\right], \tag{7.19}$$

$$\hat{\varphi}^{-+}_{\boldsymbol{K}} = \sum_{k} K^{-+}_{\boldsymbol{k}} \left[C_{\boldsymbol{nk}}(\hat{\varphi}^{-+}) + D^{-+}_{\boldsymbol{nk}}(\hat{\varphi}^{+-}, \hat{\varphi}^{-+})\right]. \tag{7.20}$$

They are coupled by

$$D^{\pm\mp}_{\boldsymbol{nk}}(\hat{\varphi}^{+-}, \hat{\varphi}^{-+}) = -\delta_{\boldsymbol{n},0} \sum_{\boldsymbol{nq}} e^{i\boldsymbol{k}\cdot(\boldsymbol{n}-\boldsymbol{n}')} \iint \hat{I}^{\pm} \hat{A}(\boldsymbol{r}_1) I^{\pm} \frac{e^2 e^{-i\boldsymbol{K}\cdot\boldsymbol{q}}}{|\boldsymbol{r}_1 - \boldsymbol{r}_2 + \boldsymbol{R}_{\boldsymbol{q}}|} \mathrm{Tr}\left(\hat{I}^{-} A(\boldsymbol{r}_2) \hat{I}^{-} \hat{\varphi}^{-+}_{\boldsymbol{K}}(0) + I^{+} A(\boldsymbol{r}_2) I^{+} \hat{\varphi}^{+-}_{\boldsymbol{K}}(0)\right) \mathrm{d}\tau_1 \mathrm{d}\tau_2 . \tag{7.21}$$

By inspection we find the symmetry

$$\hat{\varphi}^{-+}(\boldsymbol{n}) = -(\hat{\varphi}^{+-}(-\boldsymbol{n}))^{\mathrm{T}} \tag{7.22}$$

provided that we describe the direct product $\hat{\varphi}^{-+}$ by a matrix. The property (7.22) can be used to decouple the two systems (7.19) and (7.20). Both of them have the same solution with positive and negative energy differences.

§ 8. Model of an Exciton in Lowest-Order Approximation

We consider the system (7.19), which we multiply by $U_{(1)} \times U_{(2)}$. The left-hand side becomes

$$(U_{(1)} \times U_{(2)}) \hat{\varphi}^{+-}_{\boldsymbol{K}}(\boldsymbol{n}) =: \tilde{\varphi}^{+-}_{\boldsymbol{K}}(\boldsymbol{n}) = \begin{pmatrix} I & 0 \\ 0 & 0 \end{pmatrix} \tilde{\varphi}_{\boldsymbol{K}}(\boldsymbol{n}) \begin{pmatrix} 0 & 0 \\ 0 & I \end{pmatrix} = \begin{pmatrix} 0 & \varphi^{E}_{\boldsymbol{K}}(\boldsymbol{n}) \\ 0 & 0 \end{pmatrix} \tag{8.1}$$

where we have assumed, as in (7.22) that $\hat{\varphi}_{\boldsymbol{K}}(\boldsymbol{n})$ is described by a quadratic matrix

$$\tilde{\varphi}_{\boldsymbol{K}}(\boldsymbol{n}) = U \hat{\varphi}_{\boldsymbol{K}}(\boldsymbol{n}) U^{\mathrm{T}}. \tag{8.2}$$

$\varphi^{E}_{\boldsymbol{K}}(\boldsymbol{n})$ is also a matrix, which satisfies the equation

$$\begin{aligned}
\varphi^{E}_{\boldsymbol{K}}(\boldsymbol{n}) = \frac{1}{N} \sum_{n'} \sum_{\boldsymbol{k}'} e^{i\boldsymbol{k}\cdot(\boldsymbol{n}-\boldsymbol{n}')} \sum_{r=1}^{3} \iint \mathrm{d}\tau_1 \mathrm{d}\tau_2 \\
\cdot \Bigg\{ \frac{1}{\omega + \varepsilon_L(\frac{1}{2}\boldsymbol{K} + \boldsymbol{k}) - \varepsilon_V(\frac{1}{2}\boldsymbol{K} - \boldsymbol{k})} \Bigg[I_0 A(\boldsymbol{r}_1) \varphi^{E}_{\boldsymbol{K}}(\boldsymbol{n}') A(\boldsymbol{r}_2) I_r \frac{e^2}{|\boldsymbol{r}_1 - \boldsymbol{r}_2 + \boldsymbol{R}_{\boldsymbol{n}'}|} \\
- \delta_{\boldsymbol{n}',0} I_0 A(\boldsymbol{r}_1) I_r \sum_{\boldsymbol{q}} \frac{e^2 e^{-i\boldsymbol{K}\cdot\boldsymbol{q}}}{|\boldsymbol{r}_1 - \boldsymbol{r}_2 + \boldsymbol{R}_{\boldsymbol{q}}|} \mathrm{Tr}\left(A(\boldsymbol{r}_2) \varphi^{E}_{\boldsymbol{K}}(0)\right) \Bigg] \\
- \frac{1}{\omega + \varepsilon_V(\frac{1}{2}\boldsymbol{K} + \boldsymbol{k}) - \varepsilon_L(\frac{1}{2}\boldsymbol{K} - \boldsymbol{k})} \Bigg[I_r A(\boldsymbol{r}_1) \varphi^{E}_{\boldsymbol{K}}(\boldsymbol{n}') A(\boldsymbol{r}_2) I_0 \frac{e^2}{|\boldsymbol{r}_1 - \boldsymbol{r}_2 + \boldsymbol{R}_{\boldsymbol{n}'}|} \\
- \delta_{\boldsymbol{n}',0} I_r A(\boldsymbol{r}_1) I_0 \sum_{\boldsymbol{q}} \frac{e^2 e^{-i\boldsymbol{K}\cdot\boldsymbol{q}}}{|\boldsymbol{r}_1 - \boldsymbol{r}_2 + \boldsymbol{R}_{\boldsymbol{q}}|} \mathrm{Tr}\left(A(\boldsymbol{r}_2) \varphi^{E}_{\boldsymbol{K}}(0)\right) \Bigg] \Bigg\}.
\end{aligned} \tag{8.3}$$

Here r is restricted to r = 1, 2, 3. We have used

$$\begin{aligned}
\hat{I}_0^{+} \hat{A}(\boldsymbol{r}_1) \times \hat{I}_r^{-} \hat{A}(\boldsymbol{r}_2) \hat{\varphi}^{+-}(\boldsymbol{n}) = -U^{+} \begin{pmatrix} I_0 & 0 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} A(\boldsymbol{r}_1) & 0 \\ 0 & -A^{\mathrm{T}}(\boldsymbol{r}_1) \end{pmatrix} \begin{pmatrix} 0 & \varphi^{E}_{\boldsymbol{K}}(\boldsymbol{n}) \\ 0 & 0 \end{pmatrix} U^{\mathrm{H}} U \begin{pmatrix} A(\boldsymbol{r}_2) & 0 \\ 0 & -A^{r}(\boldsymbol{r}_2) \end{pmatrix} \\
\cdot \begin{pmatrix} I_r & 0 \\ 0 & 0 \end{pmatrix} U U^{\mathrm{T}} U^{\mathrm{H}} = -U^{+} \begin{pmatrix} 0 & I_0 A(\boldsymbol{r}_1) \varphi^{E}_{\boldsymbol{K}}(\boldsymbol{n}) A(\boldsymbol{r}_2) I_r \\ 0 & 0 \end{pmatrix} U^{\mathrm{H}}
\end{aligned} \tag{8.4}$$

and

$$\begin{aligned}
\mathrm{Tr}(\hat{I}^{-} \hat{A} I^{-} \hat{\varphi}^{-+}_{\boldsymbol{K}} + \hat{I}^{+} \hat{A} \hat{I}^{+} \varphi^{+-}_{\boldsymbol{K}}) = \mathrm{Tr}\Bigg(-U^{+} \begin{pmatrix} 0 & 0 \\ 0 & I \end{pmatrix} \begin{pmatrix} A & 0 \\ 0 & -A^{\mathrm{T}} \end{pmatrix} \begin{pmatrix} 0 & 0 \\ (\varphi^{E}_{\boldsymbol{K}})^{\mathrm{T}} & 0 \end{pmatrix} U^{\#} + U^{+} \begin{pmatrix} I & 0 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} A & 0 \\ 0 & -A^{\mathrm{T}} \end{pmatrix} \\
\cdot \begin{pmatrix} 0 & \varphi^{E}_{\boldsymbol{K}} \\ 0 & 0 \end{pmatrix} U^{\#} \Bigg) = \mathrm{Tr}\left((\varphi^{E}_{\boldsymbol{K}})^{\mathrm{T}} A^{\mathrm{T}} + A \varphi^{E}_{\boldsymbol{K}}\right) = 2\,\mathrm{Tr}(A \varphi^{E}_{\boldsymbol{K}})
\end{aligned} \tag{8.5}$$

(8.3) shows that $\varphi^{E}_{\boldsymbol{k}}(\boldsymbol{n})$ is composed of two parts

$$\varphi^{E}_{\boldsymbol{K}}(\boldsymbol{n}) = \chi_{\boldsymbol{K}}(\boldsymbol{n}) + \psi_{\boldsymbol{K}}(\boldsymbol{n}) \tag{8.6}$$

$$\chi_{\boldsymbol{K}}(\boldsymbol{n}) = \Lambda^L \varphi^E_{\boldsymbol{K}}(\boldsymbol{n}) \Lambda^V = \sum_r I_0 \varphi^E_{\boldsymbol{K}}(\boldsymbol{n}) I_r, \qquad \psi_{\boldsymbol{K}}(\boldsymbol{n}) = \Lambda^V \varphi^E_{\boldsymbol{K}}(\boldsymbol{n}) \Lambda^L = \sum_r I_r \varphi^E_{\boldsymbol{K}}(\boldsymbol{n}) I_0 . \tag{8.7; 8.8}$$

Therefore, (8.3) consists of two coupled systems in the variables (8.7) and (8.8). For their treatment we make some assumptions: To compute the matrix elements we choose real functions. Let $w_{\boldsymbol{n}0}(\boldsymbol{r})$ be an s-function and let $w_{\boldsymbol{n}r}(\boldsymbol{r})$ be three p-functions, whose angular part is described by spherical harmonics of first order. We also expand the Coulomb potential in spherical harmonics, and then, we get by integration of the matrix elements

$$\iint \mathrm{d}\tau_1 \, \mathrm{d}\tau_2 \, I_0 A(\boldsymbol{r}_1) I_0 \frac{e^2}{|\boldsymbol{r}_1 - \boldsymbol{r}_2 + \boldsymbol{R}_n|} I_r A(\boldsymbol{r}_2) I_{r'} = \begin{cases} \delta_{r,r'} \dfrac{e^2}{|\boldsymbol{R}_n|}\,); & \boldsymbol{n} \neq \boldsymbol{0}, \\ \delta_{r,r'} e^2 C_1\,; & C_1 > 0 \quad \boldsymbol{n} = \boldsymbol{0}, \end{cases} \tag{8.9}$$

$$\iint \mathrm{d}\tau_1 \, \mathrm{d}\tau_2 \, I_0 A(\boldsymbol{r}_1) I_r \frac{e^2}{|\boldsymbol{r}_1 - \boldsymbol{r}_2 + \boldsymbol{R}_n|} I_0 A(\boldsymbol{r}_2) I_{r'} = \begin{cases} C_0 \dfrac{e^2}{|\boldsymbol{R}_n|^5} (|\boldsymbol{R}_n|^2 \delta_{r,r'} - 3 X^r_n X^{r'}_n); & \boldsymbol{n} \neq \boldsymbol{0}, \\ \delta_{r,r'} C_2 e^2; & \boldsymbol{n} = \boldsymbol{0}; C_0 > 0, \; C_2 > 0 . \end{cases} \tag{8.10}$$

$X^r_{\boldsymbol{n}}$ are components of $\boldsymbol{R}_{\boldsymbol{n}}$

$$\iint \mathrm{d}\tau_1 \, \mathrm{d}\tau_2 \, I_0 A(\boldsymbol{r}_1) I_r \sum_{\boldsymbol{q}} \frac{e^2}{|\boldsymbol{r}_1 - \boldsymbol{r}_2 + \boldsymbol{R}_q|} \operatorname{Tr}\left(I_{r'} A(\boldsymbol{r}_1) I_0 \chi(0) + I_0 A(\boldsymbol{r}_2) I_{r'} \psi(0)\right)$$
$$= \delta_{\boldsymbol{n},0} \, \delta_{r,r'} \, e^2 C_2 \left(\chi_{0r}(0) + \psi_{r0}(0)\right). \tag{8.11}$$

In (8.11) we have used that the sum over all quadrupoles $\dfrac{\partial}{\partial X^r} \dfrac{\partial}{\partial X^{r'}} \dfrac{1}{|\boldsymbol{R}|}\Big|_{\boldsymbol{n}}$ vanishes for an ideal lattice and only one contribution is left for $\boldsymbol{q} = \boldsymbol{0}$. The constants C_0, C_1, C_2 arise from the calculation of the radial part in the chosen electronfunctions. In the case of $\boldsymbol{K} = 0$ we obtain for the various components under use of (8.9) – (8.11) the equations

$$\chi_{0r}(\boldsymbol{n}) = \sum_{\boldsymbol{n}'} g(\boldsymbol{n} - \boldsymbol{n}' \,|\, \omega) e^2$$
$$\cdot \left\{ \frac{1}{|\boldsymbol{R}_{\boldsymbol{n}'}|} \chi_{0r}(\boldsymbol{n}') + \sum_{r'} \frac{C_0}{|\boldsymbol{R}_{n'}|^5} (|\boldsymbol{R}_{\boldsymbol{n}'}|^2 - 3 X^r_{\boldsymbol{n}'} X^{r'}_{\boldsymbol{n}'}) \psi_{r'0}(\boldsymbol{n}') (1 - \delta_{\boldsymbol{n},0}) + \delta_{\boldsymbol{n},0} (C_1 - C_2) \chi_{0r}(0) \right\}, \tag{8.12}$$

$$\psi_{r0}(\boldsymbol{n}) = \sum_{\boldsymbol{n}'} g(\boldsymbol{n} - \boldsymbol{n}' \,|\, -\omega) e^2$$
$$\cdot \left\{ \frac{1}{|\boldsymbol{R}_{\boldsymbol{n}'}|} \psi_{r0}(\boldsymbol{n}') + \sum_{r'} \frac{C_0}{|\boldsymbol{R}_{\boldsymbol{n}'}|^5} (|\boldsymbol{R}_{\boldsymbol{n}'}|^2 - 3 X^r_{\boldsymbol{n}'} X^{r'}_{\boldsymbol{n}'}) \chi_{0r'}(\boldsymbol{n}') (1 - \delta_{\boldsymbol{n},0}) + \delta_{\boldsymbol{n},0} (C_1 - C_2) \psi_{r0}(0) \right\}. \tag{8.13}$$

Here we have

$$g(\boldsymbol{n} - \boldsymbol{n}' \,|\, \omega) = 1/N \sum_{k} \exp\{i \boldsymbol{k} \cdot (\boldsymbol{n} - \boldsymbol{n}')\} / (\omega + \varepsilon_L(\boldsymbol{k}) - \varepsilon_V(\boldsymbol{k})), \; \varepsilon(\boldsymbol{k}) = \varepsilon(-\boldsymbol{k}). \tag{8.14}$$

Approximations for this Green's function can be calculated by introducing approximations about lattice structure and the form $\varepsilon_L(\boldsymbol{k})$ and $\varepsilon_V(\boldsymbol{k})$. For a first inspection we omit the quadrupole coupling between $\chi(\boldsymbol{n})$ and $\psi(\boldsymbol{n})$. We recognize that in both equations an electron-hole state arises with Coulomb potential as interaction:

$$\chi_{0r}(\boldsymbol{n}) = \sum_{\boldsymbol{n}'} g(\boldsymbol{n} - \boldsymbol{n}' \,|\, \omega) (e^2 / |\boldsymbol{R}_{\boldsymbol{n}'}|) \chi_{0r}(\boldsymbol{n}'), \qquad \psi_{r0}(\boldsymbol{n}) = \sum_{\boldsymbol{n}'} g(\boldsymbol{n} - \boldsymbol{n}' \,|\, \omega) (e^2 / |\boldsymbol{R}_{\boldsymbol{n}'}|) \psi_{0r}(\boldsymbol{n}'). \tag{8.15, 8.16}$$

In an effective mass approximation for the one-electron energies (8.14) we are able to reduce (8.15) and (8.16) to a hydrogen problem [4]. The difference between these equations is merely that their solutions belong to opposite energy differences. Quadrupole coupling splits the spectral lines. But is can be shown that the whole system (8.12) and 8.13) depends only on ω^2, which we expect from the fact that the NTD-system contains pairs of solutions of ω and $-\omega$. The quadrupole terms describe a form of screening, however, it is not identical with the screening of the Coulomb potential calculated by other authors [4]. It is the next higher-order approximation that yields such an effect.

§ 9. Screening of the Coulomb Potential by Polarisation

The next approximation for the even part of (4.3) demands a break-up at $N=4$ and yields real correlations. Equation (7.1) will be completed by

$$\hat{K}(\boldsymbol{n}_1\,\boldsymbol{n}_2) := \sum_{\boldsymbol{n}\boldsymbol{n}'\boldsymbol{m}'} \hat{W}_{\boldsymbol{n}_1\boldsymbol{n}\boldsymbol{n}'\boldsymbol{m}'}\,\hat{\varphi}^4(\boldsymbol{m}'\,\boldsymbol{n}_2\,\boldsymbol{n}'\,\boldsymbol{n}) + W_{\boldsymbol{n}_2\boldsymbol{n}\boldsymbol{n}'\boldsymbol{m}'}\,\hat{\varphi}(\boldsymbol{n}_1\,\boldsymbol{m}'\,\boldsymbol{n}'\,\boldsymbol{n}) \tag{9.1}$$

$$\approx \sum_{\boldsymbol{n}'}\iint \mathrm{d}\tau_3\,\mathrm{d}\tau_4\left(\hat{A}_{\boldsymbol{n}_1\boldsymbol{n}_1}(\boldsymbol{r}_3)\frac{e^2}{|\boldsymbol{r}_3-\boldsymbol{r}_4|}\hat{A}_{\boldsymbol{n}'\boldsymbol{n}'}(\boldsymbol{r}_4)\,\hat{\varphi}^4(\boldsymbol{n}_1\,\boldsymbol{n}_2\boldsymbol{n}'\,\boldsymbol{n}') + \hat{A}_{\boldsymbol{n}_2\boldsymbol{n}_2}(\boldsymbol{r}_3)\frac{e^2}{|\boldsymbol{r}_3-\boldsymbol{r}_4|}\hat{A}_{\boldsymbol{n}'\boldsymbol{n}'}(\boldsymbol{r}_4)\,\hat{\varphi}^4(\boldsymbol{n}_1\,\boldsymbol{n}_2\boldsymbol{n}'\,\boldsymbol{n}')\right).$$

The latter holds with (7.4). Refering back to (7.9) we are interested in the projection

$$\hat{K}^{+-}(\boldsymbol{n}_1\,\boldsymbol{n}_2) = (\hat{I}^{+}_{(1)}\times\hat{I}^{-}_{(2)})\hat{K}(\boldsymbol{n}_1\,\boldsymbol{n}_2). \tag{9.2}$$

The components φ^4 in (9.1) are determined by (6.4) with $k=4$. We note, that the coupling to φ^6 is cut off by the truncation at $N=4$. In particular we find

$$\hat{\varphi}^4(\boldsymbol{n}_1\,\boldsymbol{n}_2\,\boldsymbol{n}_3\,\boldsymbol{n}_4) = \sum_{\boldsymbol{n}_1'\ldots\boldsymbol{n}_4'} \hat{G}(\boldsymbol{n}_1-\boldsymbol{n}_1',\ldots\boldsymbol{n}_4-\boldsymbol{n}_4'\,|\,\omega)\,\hat{R}^{(\mathrm{a})}(\boldsymbol{n}_1'\ldots\boldsymbol{n}_4'). \tag{9.3}$$

$R^{(\mathrm{a})}$ contains only the coupling to $\hat{\varphi}^4$ and $\hat{\varphi}^2$. For a first treatment it may be enough to take along such terms, which give a coupling to the $\hat{\varphi}^2$'s. There remains the following part

$$\begin{aligned}\hat{R}^{(\mathrm{a})} \approx \hat{R}^{(\mathrm{b})}(\boldsymbol{n}_1\ldots\boldsymbol{n}_4) &= \\ &= \sum_{ijj'=1}^{4}\sum_{\boldsymbol{m}'}\left[2\,\hat{F}_{\boldsymbol{n}_i}\hat{F}_{\boldsymbol{n}_j}\hat{W}_{\boldsymbol{n}_i\boldsymbol{n}_j\boldsymbol{n}_{j'}\boldsymbol{m}'} - \hat{F}_{\boldsymbol{n}_j}\hat{W}_{\boldsymbol{n}_i\boldsymbol{n}_j\boldsymbol{n}_{j'}\boldsymbol{m}'}\hat{F}_{\boldsymbol{n}_{j'}} + \tfrac{1}{4}\hat{W}_{\boldsymbol{n}_i\boldsymbol{n}_j\boldsymbol{n}_{j'}\boldsymbol{m}'}\right](-1)^{P_{jj'}}\hat{\varphi}^2\,(\ldots\boldsymbol{m}'/i\ldots) \\ &= 8\sum_{ijj'=1}^{4}\sum_{\boldsymbol{m}'}\iint \mathrm{d}\tau_1\,\mathrm{d}\tau_2\Big(\hat{\Lambda}^L_{\boldsymbol{n}_j}\hat{A}_{\boldsymbol{n}_j\boldsymbol{n}_{j'}}(\boldsymbol{r}_1)\hat{\Lambda}^V_{\boldsymbol{n}_{j'}}\frac{e^2}{|\boldsymbol{r}_1-\boldsymbol{r}_2|}\hat{\Lambda}^L_{\boldsymbol{n}_i}\hat{A}_{\boldsymbol{n}_i\boldsymbol{m}'}(\boldsymbol{r}_2) + \\ &\quad + \hat{\Lambda}^V_{\boldsymbol{n}_j}\hat{A}_{\boldsymbol{n}_j\boldsymbol{n}_{j'}}(\boldsymbol{r}_1)\hat{\Lambda}^L_{\boldsymbol{n}_{j'}}\frac{e^2}{|\boldsymbol{r}_1-\boldsymbol{r}_2|}\hat{\Lambda}^V_{\boldsymbol{n}_i}\hat{A}_{\boldsymbol{n}_i\boldsymbol{m}'}(\boldsymbol{r}_2)\Big)(-1)^{P_{jj'}}\hat{\varphi}^2\,(\ldots\boldsymbol{m}'/i\ldots).\end{aligned} \tag{9.4}$$

(9.4) contains twelve terms without counting the permutations. An analysis shows that only two terms cover long-range interactions in $|\boldsymbol{n}_1-\boldsymbol{n}_2|$. With respect to (7.4) they are summarized by

$$\begin{aligned}\hat{R}^{(W)}(\boldsymbol{n}_1\,\boldsymbol{n}_2\,\boldsymbol{n}_3\,\boldsymbol{n}_4) = 16\iint \mathrm{d}\tau_1\,\mathrm{d}\tau_2\Big(&\hat{\Lambda}^L_{\boldsymbol{n}_3}\hat{A}_{\boldsymbol{n}_3\boldsymbol{n}_4}(\boldsymbol{r}_1)\hat{\Lambda}^V_{\boldsymbol{n}_4}\frac{e^2}{|\boldsymbol{r}_1-\boldsymbol{r}_2|}\left(\hat{\Lambda}^L_{\boldsymbol{n}_1}\hat{A}_{\boldsymbol{n}_1\boldsymbol{n}_1}(\boldsymbol{r}_2) + \hat{\Lambda}^L_{\boldsymbol{n}_2}A_{\boldsymbol{n}_2\boldsymbol{n}_2}(\boldsymbol{r}_2)\right) + \\ &+ \hat{\Lambda}^V_{\boldsymbol{n}_3}\hat{A}_{\boldsymbol{n}_3\boldsymbol{n}_4}(\boldsymbol{r}_1)\hat{\Lambda}^L_{\boldsymbol{n}_4}\frac{e^2}{|\boldsymbol{r}_1-\boldsymbol{r}_2|}\left(\hat{\Lambda}^V_{\boldsymbol{n}_1}\hat{A}_{\boldsymbol{n}_1\boldsymbol{n}_1}(\boldsymbol{r}_2) + \hat{\Lambda}^V_{\boldsymbol{n}_2}\hat{A}_{\boldsymbol{n}_2\boldsymbol{n}_2}(\boldsymbol{r}_2)\right)\Big)\,\hat{\varphi}^2(\boldsymbol{n}_1\,\boldsymbol{n}_2)\,\delta_{\boldsymbol{n}_3\boldsymbol{n}_4}.\end{aligned} \tag{9.5}$$

According to (9.3) the next step is the application of the Green's function (6.10) upon (9.5) and the computation of the projection (9.2) with the aid of (7.8). By use of symmetries we get an expression for the long-range interaction (without self-energy terms) of the form

$$\begin{aligned}\hat{K}^{(W)+-}_{(\boldsymbol{n}_1\boldsymbol{n}_2)} = &\frac{-1}{N^4}\sum_{\substack{k_1\ldots k_4\\ \boldsymbol{n}_1'\ldots\boldsymbol{n}_4',\,\boldsymbol{n}'}} 8\,e^4\,\delta_{\boldsymbol{n}_3',\,\boldsymbol{n}_4'}\iiiint\frac{e^{i[\boldsymbol{k}_1\cdot(\boldsymbol{n}_1-\boldsymbol{n}_1')+\boldsymbol{k}_2\cdot(\boldsymbol{n}_2-\boldsymbol{n}_2')+(\boldsymbol{k}_3+\boldsymbol{k}_4)\cdot(\boldsymbol{n}'-\boldsymbol{n}_3)]}}{|\boldsymbol{r}_1-\boldsymbol{r}_2|\,|\boldsymbol{r}_3-\boldsymbol{r}_4|} \\ &\cdot\sum_{r=1}^{3}\mathrm{Tr}\left(\hat{A}_{\boldsymbol{n}'\boldsymbol{n}'}(\boldsymbol{r}_4)\hat{I}_0{}^{+}A_{\boldsymbol{n}_3'\boldsymbol{n}_3'}(\boldsymbol{r}_4)\hat{I}^{+}_r\right) + \sum_{l_1l_2=1}^{3}\Bigg\{\frac{\hat{I}_0{}^{+}\hat{A}_{\boldsymbol{n}_1'\boldsymbol{n}_1'}(\boldsymbol{r}_2)\hat{I}^{+}_{l_1}\hat{\varphi}^{+-}_{(\boldsymbol{n}_1'\boldsymbol{n}_2')}\hat{I}^{+}_{l_2}\hat{A}_{\boldsymbol{n}_2\boldsymbol{n}_2}(\boldsymbol{r}_3)\hat{I}^{+}}{\omega+\varepsilon_L(1)-\varepsilon_{l_2}(2)+\varepsilon_L(3)-\varepsilon_V(4)} \\ &+\sum_r\frac{\hat{I}^{+}\hat{A}_{\boldsymbol{n}_1\boldsymbol{n}_1}(\boldsymbol{r}_3)\hat{I}^{+}_{l_1}\hat{\varphi}^{+-}(\boldsymbol{n}_1'\,\boldsymbol{n}_2')\hat{I}^{+}_{l_2}\hat{A}_{\boldsymbol{n}_1'\boldsymbol{n}_2'}(\boldsymbol{r}_2)\hat{I}_r{}^{+}}{\omega+\varepsilon_{l_1}(1)-\varepsilon_V(2)+\varepsilon_L(3)-\varepsilon_V(4)} + \sum_r\frac{\hat{I}_r{}^{+}\hat{A}_{\boldsymbol{n}_1'\boldsymbol{n}_1'}(\boldsymbol{r}_2)\,\hat{I}^{+}_{l_1}\hat{\varphi}^{+-}(\boldsymbol{n}_1'\,\boldsymbol{n}_2')\hat{I}^{+}_{l_2}\hat{A}_{\boldsymbol{n}_2\boldsymbol{n}_2}(\boldsymbol{r}_3)\hat{I}^{+}}{\omega+\varepsilon_V(1)-\varepsilon_{l_2}(2)+\varepsilon_V(3)-\varepsilon_L(4)} \\ &+\frac{\hat{I}^{+}A_{\boldsymbol{n}_1\boldsymbol{n}_1}(\boldsymbol{r}_3)\hat{I}^{+}_{l_1}\hat{\varphi}^{+-}(\boldsymbol{n}_1'\,\boldsymbol{n}_2')\hat{I}^{+}_{l_2}\hat{A}_{\boldsymbol{n}_2'\boldsymbol{n}_2'}(\boldsymbol{r}_2)\hat{I}_0{}^{+}}{\omega+\varepsilon_{l_1}(1)-\varepsilon_L(2)+\varepsilon_V(3)-\varepsilon_L(4)}\Bigg\}\,\mathrm{d}\tau_1\ldots\mathrm{d}\tau_4; \quad \varepsilon(i)\equiv\varepsilon(\boldsymbol{k}_i),\quad i=1,2,3,4.\end{aligned} \tag{9.6}$$

(9.6) may be evaluated with the aid of those kinds of considerations, which produced the results (8.9) – (8.11). We want to take into account only such terms which contribute pole terms in the brackets

of (9.6), and in the trace term we keep a product of two dipoles. One can write the result in the following form

$$\hat{K}^{(W)+-}(\boldsymbol{n}_1\,\boldsymbol{n}_2) = -\frac{8\,e^4\,C_0{}^2}{N^4}\sum_{\substack{\boldsymbol{k}_1\ldots\boldsymbol{k}_4\\ \boldsymbol{n}_1'\ldots\boldsymbol{n}_4',\boldsymbol{n}'}}\delta_{\boldsymbol{n}_3',\boldsymbol{n}_4'}\exp\{i[\boldsymbol{k}_1\cdot(\boldsymbol{n}_1-\boldsymbol{n}_1')+\boldsymbol{k}_2\cdot(\boldsymbol{n}_2-\boldsymbol{n}_2')+(\boldsymbol{k}_3+\boldsymbol{k}_4)\cdot(\boldsymbol{n}'-\boldsymbol{n}_3')]\}$$

$$\cdot\Bigg\{\frac{(\boldsymbol{R}_{\boldsymbol{n}_3'}-\boldsymbol{R}_{\boldsymbol{n}_1'})\cdot(\boldsymbol{R}_{\boldsymbol{n}_2}-\boldsymbol{R}_{\boldsymbol{n}'})}{|\boldsymbol{R}_{\boldsymbol{n}_3'}-\boldsymbol{R}_{\boldsymbol{n}_1'}|\,|\boldsymbol{R}_{\boldsymbol{n}_2}-\boldsymbol{R}_{\boldsymbol{n}'}|}\Bigg(\sum_{l_2}\frac{(\hat{I}_0{}^+\times\hat{I}_{l_2}{}^-)\,\hat{\varphi}^{+-}(\boldsymbol{n}_1'\,\boldsymbol{n}_2')}{\omega+\varepsilon_L(1)-\varepsilon_{l_2}(2)+\varepsilon_L(3)-\varepsilon_V(4)}$$

$$+\sum_{r,l_2}\frac{(\hat{I}_r{}^+\times\hat{I}_{l_2})\,\hat{\varphi}^{+-}(\boldsymbol{n}_1'\,\boldsymbol{n}_2')}{\omega+\varepsilon_V(1)-\varepsilon_{l_2}(2)+\varepsilon_V(3)-\varepsilon_L(4)}\Bigg)+\frac{(\boldsymbol{R}_{\boldsymbol{n}_3'}-\boldsymbol{R}_{\boldsymbol{n}_2'})\cdot(\boldsymbol{R}_{\boldsymbol{n}_1}-\boldsymbol{R}_{\boldsymbol{n}'})}{|\boldsymbol{R}_{\boldsymbol{n}_3'}-\boldsymbol{R}_{\boldsymbol{n}_2'}|\,|\boldsymbol{R}_{\boldsymbol{n}_1}-\boldsymbol{R}_{\boldsymbol{n}'}|}$$

$$\cdot\Bigg(\sum_{l_1,r}\frac{(\hat{I}_{l_1}{}^+\times\hat{I}_r{}^-)\,\hat{\varphi}^{+-}(\boldsymbol{n}_1'\,\boldsymbol{n}_2')}{\omega+\varepsilon_{l_1}(1)-\varepsilon_V(2)+\varepsilon_L(3)-\varepsilon_V(4)}+\sum_{l_1}\frac{(\hat{I}_{l_1}{}^+\times\hat{I}_0{}^-)\,\hat{\varphi}^{+-}(\boldsymbol{n}_1'\,\boldsymbol{n}_2')}{\omega+\varepsilon_{l_1}(1)-\varepsilon_L(2)+\varepsilon_V(3)-\varepsilon_L(4)}\Bigg)\Bigg\}. \tag{9.7}$$

Since we are interested in completing the Eqs. (8.15) and (8.16) the terms

$$\chi_{0r}=(U\times U)\,(\hat{I}_0{}^+\times\hat{I}_r{}^-)\hat{\varphi}^{+-}\quad\text{and}\quad\psi_{r0}=(U\times U)\,(\hat{I}_r{}^+\times\hat{I}_0{}^-)\hat{\varphi}^{+-} \tag{9.8}$$

become relevant. Therefore, the Coulomb interaction on the right-hand side of (8.15) will be supplemented by the term

$$\hat{K}^{(W)+-}_{0\ r}(\boldsymbol{n}_1\,\boldsymbol{n}_2) = -\frac{8\,e^4\,C_0{}^2}{N^4}\sum_{\substack{k_1\ldots k_4\\ \boldsymbol{n}_1'\ldots\boldsymbol{n}_4',\boldsymbol{n}'}}\delta_{\boldsymbol{n}_3',\boldsymbol{n}_4}\frac{\exp\{i[\boldsymbol{k}_1\cdot(\boldsymbol{n}_1-\boldsymbol{n}_1')+\boldsymbol{k}_2\cdot(\boldsymbol{n}_2-\boldsymbol{n}_2')+(\boldsymbol{k}_3+\boldsymbol{k}_4)\cdot(\boldsymbol{n}'-\boldsymbol{n}_3')]\}}{\omega+\varepsilon_L(1)-\varepsilon_V(2)+\varepsilon_L(3)-\varepsilon_V(4)}$$

$$\cdot\Bigg\{\frac{(\boldsymbol{R}_{\boldsymbol{n}_3'}-\boldsymbol{R}_{\boldsymbol{n}_1'})\cdot(\boldsymbol{R}_{\boldsymbol{n}_2}-\boldsymbol{R}_{\boldsymbol{n}'})}{|\boldsymbol{R}_{\boldsymbol{n}_3'}-\boldsymbol{R}_{\boldsymbol{n}_1'}|\,|\boldsymbol{R}_{\boldsymbol{n}_2}-\boldsymbol{R}_{\boldsymbol{n}'}|}+\frac{(\boldsymbol{R}_{\boldsymbol{n}_3'}-\boldsymbol{R}_{\boldsymbol{n}_2'})\cdot(\boldsymbol{R}_{\boldsymbol{n}_1}-\boldsymbol{R}_{\boldsymbol{n}'})}{|\boldsymbol{R}_{\boldsymbol{n}_3'}-\boldsymbol{R}_{\boldsymbol{n}_2'}|\,|\boldsymbol{R}_{\boldsymbol{n}_1}-\boldsymbol{R}_{\boldsymbol{n}'}|}\Bigg\}\chi_{0r}(\boldsymbol{n}_1'\,\boldsymbol{n}_2') \tag{9.9}$$

and (8.16) by the same expression with $-\omega$ instead of ω. To evaluate (9.9) we make some substitutions

$$\boldsymbol{n}_1'=\boldsymbol{n}_1-\boldsymbol{p};\quad \boldsymbol{n}_2'=\boldsymbol{n}_2-\boldsymbol{q};\quad \boldsymbol{n}_3'=\boldsymbol{n}'-\boldsymbol{m}. \tag{9.10}$$

Then we get

$$K^{(W)+-}_{0\ r}(\boldsymbol{n}_1\,\boldsymbol{n}_2) = -\frac{8\,e^4\,C_0{}^2}{N^4}\sum_{k_1\ldots k_4}\sum_{\boldsymbol{p}\boldsymbol{q}\boldsymbol{m}}\frac{\exp\{i[\boldsymbol{k}_1\cdot\boldsymbol{p}+\boldsymbol{k}_2\cdot\boldsymbol{q}+(\boldsymbol{k}_3+\boldsymbol{k}_4)\cdot\boldsymbol{m}]\}}{\omega+\varepsilon_L(1)-\varepsilon_V(2)+\varepsilon_L(3)-\varepsilon_V(4)} \tag{9.11}$$

$$\cdot\sum_{\boldsymbol{n}'}\Bigg\{\frac{(\boldsymbol{R}_{\boldsymbol{n}'}-\boldsymbol{R}_{\boldsymbol{m}}-\boldsymbol{R}_{\boldsymbol{n}_1}+\boldsymbol{R}_{\boldsymbol{p}})\cdot(\boldsymbol{R}_{\boldsymbol{n}_2}-\boldsymbol{R}_{\boldsymbol{n}'})}{|\boldsymbol{R}_{\boldsymbol{n}'}-\boldsymbol{R}_{\boldsymbol{m}}-\boldsymbol{R}_{\boldsymbol{n}_1}+\boldsymbol{R}_{\boldsymbol{p}}|\,|\boldsymbol{R}_{\boldsymbol{n}_2}-\boldsymbol{R}_{\boldsymbol{n}'}|}+\frac{(\boldsymbol{R}_{\boldsymbol{n}'}-\boldsymbol{R}_{\boldsymbol{m}}-\boldsymbol{R}_{\boldsymbol{n}_2}-\boldsymbol{R}_{\boldsymbol{q}})\cdot(\boldsymbol{R}_{\boldsymbol{n}_1}-\boldsymbol{R}_{\boldsymbol{n}'})}{|\boldsymbol{R}_{\boldsymbol{n}'}-\boldsymbol{R}_{\boldsymbol{m}}-\boldsymbol{R}_{\boldsymbol{n}_2}-\boldsymbol{R}_{\boldsymbol{q}}|\,|\boldsymbol{R}_{\boldsymbol{n}_1}-\boldsymbol{R}_{\boldsymbol{n}'}|}\Bigg\}\chi_{0r}(\boldsymbol{n}_1-\boldsymbol{p},\boldsymbol{n}_2-\boldsymbol{q}).$$

The sum over $\boldsymbol{n}'$ in the brackets of (9.11) can be mastered by passing over to integrals and using the properties of potential functions [7]. The result is

$$\sum_{\boldsymbol{n}'}\frac{(\boldsymbol{R}_{\boldsymbol{n}'}-\boldsymbol{R}_{\boldsymbol{a}})\cdot(\boldsymbol{R}_{\boldsymbol{b}}-\boldsymbol{R}_{\boldsymbol{n}'})}{|\boldsymbol{R}_{\boldsymbol{n}'}-\boldsymbol{R}_{\boldsymbol{a}}|\,|\boldsymbol{R}_{\boldsymbol{b}}-\boldsymbol{R}_{\boldsymbol{n}'}|}\approx\frac{4\pi}{d^3}\frac{1}{|\boldsymbol{R}_{\boldsymbol{a}}-\boldsymbol{R}_{\boldsymbol{b}}|}, \tag{9.12}$$

d = distance between nearest neighbor ions.

We transform to centre-of-mass coordinates and use

$$\begin{aligned}&\boldsymbol{N}=\tfrac{1}{2}(\boldsymbol{n}_1+\boldsymbol{n}_2);\quad \boldsymbol{n}=(\boldsymbol{n}_1-\boldsymbol{n}_2);\quad \boldsymbol{S}=\tfrac{1}{2}(\boldsymbol{p}+\boldsymbol{q});\quad \boldsymbol{s}=(\boldsymbol{p}-\boldsymbol{q}),\\ &\boldsymbol{K}'=(\boldsymbol{k}_1+\boldsymbol{k}_2);\quad \boldsymbol{k}'=\tfrac{1}{2}(\boldsymbol{k}_1-\boldsymbol{k}_2);\quad \boldsymbol{K}''=(\boldsymbol{k}_3+\boldsymbol{k}_4);\quad \boldsymbol{k}''+\tfrac{1}{2}(\boldsymbol{k}_3-\boldsymbol{k}_4),\end{aligned} \tag{9.13}$$

and the Fourier representations

$$K^{(W)+-}(\boldsymbol{n}_1\,\boldsymbol{n}_2)=-\frac{1}{\sqrt{N}}\sum_{\boldsymbol{K}}K^{(w)}_{\boldsymbol{K}}(\boldsymbol{n})\,e^{\boldsymbol{K}\cdot\boldsymbol{N}};\quad \chi(\boldsymbol{n}_1-\boldsymbol{p},\boldsymbol{n}_2-\boldsymbol{q})=\frac{1}{\sqrt{N}}\sum_{\boldsymbol{K}}\chi_{\boldsymbol{K}}(\boldsymbol{n}-\boldsymbol{s})\,e^{i\boldsymbol{K}(\boldsymbol{N}-\boldsymbol{S})}. \tag{9.14}$$

(9.14) yields

$$K^{(W)}_{\boldsymbol{K}}(\boldsymbol{n})=-\frac{8\,e^4\,C_0{}^2}{N^4}\frac{4\pi}{d^3}\sum_{\boldsymbol{K}'\boldsymbol{K}''\boldsymbol{k}'\boldsymbol{k}''}\sum_{\boldsymbol{S}\boldsymbol{s}\boldsymbol{m}}\exp\{i[\boldsymbol{K}'\cdot\boldsymbol{S}+\boldsymbol{k}'\cdot\boldsymbol{s}+\boldsymbol{K}''\cdot\boldsymbol{m}-\boldsymbol{K}\cdot\boldsymbol{S}]\}\Bigg(\frac{1}{|\boldsymbol{R}_{\boldsymbol{n}}-\boldsymbol{R}_{\boldsymbol{m}}-\boldsymbol{R}_{\boldsymbol{S}}-\frac{1}{2}\boldsymbol{R}_{\boldsymbol{s}}|}$$

$$\cdot+\frac{1}{|\boldsymbol{R}_{\boldsymbol{n}}-\boldsymbol{R}_{\boldsymbol{m}}+\boldsymbol{R}_{\boldsymbol{S}}-\frac{1}{2}\boldsymbol{R}_{\boldsymbol{s}}|}\Bigg)\frac{\chi_{\boldsymbol{K}}(\boldsymbol{n}-\boldsymbol{s})}{\omega+\varepsilon_L(\tfrac{1}{2}\boldsymbol{K}'+\boldsymbol{k}')-\varepsilon_V(\tfrac{1}{2}\boldsymbol{K}'-\boldsymbol{k}')+\varepsilon_L(\tfrac{1}{2}\boldsymbol{K}''+\boldsymbol{k}'')-\varepsilon_V(\tfrac{1}{2}\boldsymbol{K}''-\boldsymbol{k}'')}. \tag{9.15}$$

By restriction to $\boldsymbol{K}=0$ we get with the Fourier representation of the Coulomb potential

$$1/|\boldsymbol{R}_{\boldsymbol{n}}| = (4\pi/d^3 N) \sum_{\boldsymbol{k}} e^{i\boldsymbol{k}\boldsymbol{n}}/|\boldsymbol{k}|^2 \tag{9.16}$$

and with the additional substitutions

$$\boldsymbol{M}=\tfrac{1}{2}(\boldsymbol{m}+\boldsymbol{S}); \quad \boldsymbol{P}=\boldsymbol{K}'+\boldsymbol{K}''; \quad \boldsymbol{L}=\tfrac{1}{2}(\boldsymbol{K}'-\boldsymbol{K}''), \tag{9.17}$$

the following expression

$$K^{(W)}_{0r}(\boldsymbol{n}) = -\frac{4\pi}{d^3}\frac{16\,e^4 C_0^{\,2}}{N^3}\sum_{\boldsymbol{L}\boldsymbol{k}'\boldsymbol{k}''\boldsymbol{s}} \frac{1}{|\boldsymbol{L}|^2}\,\frac{\cos L\cdot(\boldsymbol{n}-\tfrac{1}{2}\boldsymbol{s})\,\chi_{0r}(\boldsymbol{n}-\boldsymbol{s})\,e^{i\boldsymbol{k}''\cdot\boldsymbol{s}}}{\omega+\varepsilon_L(\tfrac{1}{2}\boldsymbol{L}+\boldsymbol{k}')-\varepsilon_V(\tfrac{1}{2}\boldsymbol{L}-\boldsymbol{k}')+\varepsilon_L(\tfrac{1}{2}\boldsymbol{L}-\boldsymbol{k}'')-\varepsilon_V(\tfrac{1}{2}\boldsymbol{L}+\boldsymbol{k}'')}\,. \tag{9.18}$$

In $\boldsymbol{L}$ we have to sum over the whole reciprocal lattice, while the summation over $\boldsymbol{k}'$ and $\boldsymbol{k}''$ covers only a basic cell in the reciprocal lattice.

For reason of simplicity we do not want to diagonalisize the whole problem (8.15) plus (9.18), but calculate (9.18) just for $\boldsymbol{s}=0$. In addition we assume for the energies ε_L and ε_V only next-neighbour-interaction in the cubic primitive lattice. In this case

$$\varepsilon_L(\boldsymbol{k}) = \varepsilon_L(0) - a^2\sum_{i=1}^{3}\cos k_i d\,; \quad \varepsilon_V(\boldsymbol{k}) = \varepsilon_V(0) + b^2\sum_{i=1}^{3}\cos k_i d\,. \tag{9.19}$$

We define $\Delta=\varepsilon_L(0)-\varepsilon_V(0)$ and choose for simplicity $b=a$. By changing the summations to integrations, we get

$$K^{(W)}_{0r}(\boldsymbol{n}) \approx -\left(\frac{4\pi}{d^3}\right)^2\frac{16\,e^4 C_0^{\,2} d^2}{(2\pi)^9}\int_{-\pi}^{\pi}\mathrm{d}^3\varphi\int_{-\pi}^{\pi}\mathrm{d}^3\varphi'\int_{-\infty}^{\infty}\mathrm{d}\boldsymbol{x}\,\frac{1}{|\boldsymbol{x}|^2}\,\frac{\cos\left(\frac{1}{d}\,\boldsymbol{x}\cdot\boldsymbol{n}\right)\chi_{0r}(\boldsymbol{n})}{\omega+2\Delta-2a^2\sum_{i=1}^{3}\cos\tfrac{1}{2}x_i(\cos\varphi_i+\cos\varphi_i')} \tag{9.20}$$

To recognize the law of interaction for the distance $|\boldsymbol{n}|=n$, we use for the integrations in φ and φ' the average value theorem of calculus. Employing symmetry properties we find

$$K^{(W)}_{0r}(\boldsymbol{n}) \approx -\frac{32\,e^4 C_0^{\,2}}{d^4\pi}\int_{-\infty}^{\infty}\mathrm{d}\boldsymbol{x}\,\frac{1}{|\boldsymbol{x}|^2}\,\frac{\cos\left(\frac{1}{d}\,\boldsymbol{x}\cdot\boldsymbol{n}\right)\chi_{0r}(\boldsymbol{n})}{\omega+2\Delta-4a^2\cos\xi\,(\sum_i\cos\tfrac{1}{2}x_i)} \tag{9.21}$$

Here ξ is a value in the closed interval $[-\pi,\pi]$. We choose the approximation $\sum_i \cos\tfrac{1}{2}x_i = 3-\tfrac{1}{4}\boldsymbol{x}^2$ and then we are able to integrate (9.21) in spherical coordinates

$$K^{(W)}_{0r}(\boldsymbol{n}) \approx -\frac{32\,e^4 C_0^{\,2}\pi\,\chi_{0r}(\boldsymbol{n})}{d^3(\omega+2\Delta-12\,a^2\cos\xi)}\,\frac{1}{|\boldsymbol{n}|}\left(1-\exp\left(-|\boldsymbol{n}|\sqrt{\frac{\omega+2\Delta-12\,a^2\cos\xi}{a^2\cos\xi}}\right)\right). \tag{9.22}$$

Thus, the additional interaction term (9.22) screens the Coulomb potential in the case of long-range distances. For short distances it approaches a constant exponentially [8].

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