A Practical Method to Derive Canonical Transformations in a Closed Form and it's Application to an Antiresonant Electron-Phonon-System

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A practical method for the calculation of canonical exponential transformations in closed analytic forms is presented. An application to an antiresonant electron-phonon system is given. In particular the optical zero phonon line is calculated, which reflects the resonant nature of the system.

I. Introduction

In many theoretical problems of quantum-mechanics the application of canonical transformations is desirable. A very elegant and effective technique is given by the exponential transformation method. However, in most of the nontrivial cases the treatment of the transformation is very cumbersome since each single operator of the system must be expanded in a series of commutators. The different series then have to be summed up into a closed form and therefore their generating laws must be known.

In this article we derive a method which allows a systematic calculation of transformed operators (or operator products) in an analytic form. Using a little trick the complicated summation problem can be transferred to a system of differential equations, which need to be solved. For these further calculations all well-known mathematical techniques for handling differential equations can be used.

For an illustration we apply this method to an antiresonant electron-phonon system. In two limiting cases the Hamiltonian can be diagonalized exactly. In addition the zero phonon line of the optical absorption spectrum is discussed in dependence of the coupling parameters.

2. The Differential-Equation-Method

We consider the transformation

$$\tilde{\tilde{\hat{O}}} = \hat{U}^{-1}\,\hat{O}\,\hat{U}; \quad \hat{U} = \exp[-\hat{S}]\,, \tag{1}$$

where the exponential $\hat{S}$ may be found by different techniques[1, 2]. Each single operator $\hat{O}$ of the system has to be transformed $\tilde{\tilde{\hat{O}}} = \hat{U}^{-1}\,\hat{O}\,\hat{U} = e^{-\hat{S}}\,\hat{O}\,e^{\hat{S}}$. The usual way to calculate the operator in the new basis is to expand Expr. (1) in a commutator series:

$$e^{-\hat{S}}\,\hat{O}\,e^{\hat{S}} = \hat{O} + [\hat{O}, \hat{S}] + \frac{1}{2!}[[\hat{O}, \hat{S}], \hat{S}] + \dots\,. \tag{2}$$

In nontrivial cases the summation of this series expansion is very cumbersome and often impossible. To resolve these difficulties we introduce a factor λ in the exponent of the transformation

$$(\hat{U} \to \exp[-\lambda\,\hat{S}])\,.$$

At the end of the calculation the parameter λ must be set equal to one. We differentiate the transformed operator $\tilde{\tilde{\hat{O}}}(\lambda)$ with respect to λ and get

$$\frac{\partial}{\partial\lambda}\,\tilde{\tilde{\hat{O}}}(\lambda) = e^{-\lambda\hat{S}}\,[\hat{O}, \hat{S}]\;e^{\lambda\hat{S}} = [\tilde{\tilde{\hat{O}}}, \tilde{\tilde{\hat{S}}}]\,, \tag{3}$$

where $\tilde{\tilde{\hat{S}}} = \hat{S}$. If the operator $[\tilde{\tilde{\hat{O}}}, \tilde{\tilde{\hat{S}}}]$ depends not only on the operator $\tilde{\tilde{\hat{O}}}$, but also on further operators $\tilde{\tilde{\hat{F}}}$, $\tilde{\tilde{\hat{G}}}$ ..., we have to derive differential-equations also for the operators $\tilde{\tilde{\hat{F}}}$, $\tilde{\tilde{\hat{G}}}$ ... and so on. In this way one gets a system of differential-equations:

$$\begin{aligned}
\frac{\partial}{\partial\lambda}\,\tilde{\tilde{\hat{O}}} &= [\tilde{\tilde{\hat{O}}}, \tilde{\tilde{\hat{S}}}] = \mathfrak{o}\,(\tilde{\tilde{\hat{O}}}, \tilde{\tilde{\hat{F}}}, \tilde{\tilde{\hat{G}}}, \dots)\,,\\
\frac{\partial}{\partial\lambda}\,\tilde{\tilde{\hat{F}}} &= [\tilde{\tilde{\hat{F}}}, \tilde{\tilde{\hat{S}}}] = \mathfrak{f}\,(\tilde{\tilde{\hat{O}}}, \tilde{\tilde{\hat{F}}}, \tilde{\tilde{\hat{G}}}, \dots)\,,\\
\frac{\partial}{\partial\lambda}\,\tilde{\tilde{\hat{G}}} &= [\tilde{\tilde{\hat{G}}}, \tilde{\tilde{\hat{S}}}] = \mathfrak{g}\,(\tilde{\tilde{\hat{O}}}, \tilde{\tilde{\hat{F}}}, \tilde{\tilde{\hat{G}}}, \dots)\,.\\
&\text{— — —} \qquad \text{— — —} \qquad \text{— — —}
\end{aligned} \tag{4}$$

Inserting subsequently one equation into another, an uncoupled differential-equation for any specific operator (or operator product) can be found. This equation may be of first or higher order in the derivatives $\partial/\partial\lambda$. It's general solution will have one

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or more free constants available, which must be determined. They can be calculated by expanding the solution in orders of λ and comparing with the corresponding orders of the commutator series expansion (2). Then, obviously the number of orders which have to be taken into account (inclusive the zeroth order) must be equal to the number of free constants.

3. Application to an Antiresonant Electron-Phonon System

We shall illustrate the differential-equation method at a system, which consists of two electronically coupled impurity centres (labeled 1 and 2). One of them (centre 1) interacts with the vibrations of the surrounding crystal. Examples of such a situation are found in the optical spectrum of V^{2+} in octahedral fluoride coordination[3]. They are characterized by the Hamiltonian[4, 5] ($\hbar = 1$)

$$H = \varepsilon_1 a_1^+ a_1 + \varepsilon_2 a_2^+ a_2 + v(a_1^+ a_2 + a_2^+ a_1) + a_1^+ a_1 \sum_j K_j (b_j^+ + b_j) + \sum_i \omega_i b_i^+ b_i , \tag{5}$$

where a_i^+, a_i (fermions) are the electronic and b_i^+, b_i (bosons) the vibrational creation- and annihilation operators. ε_1, ε_2 and ω_i are the energies of the uncoupled electron and phonon states. K_j indicates the electron-phonon coupling strength *.

With the help of the U-matrix formalism[1] we may derive a canonical exponential transformation for the Hamiltonian (5) with the exponent

$$\hat{S} = -\xi (a_1^+ a_2 - a_2^+ a_1) - a_1^+ a_1 \sum_j \eta_j (b_j^+ - b_j) \tag{6}$$

ξ and η_j are parameters which are given by[1, 4]

$$\xi = v/(\varepsilon_1 - \varepsilon_2) , \quad \eta_j = K_j/\omega_j . \tag{7}$$

In the following, however, we take them as free parameters, which are determined later. To calculate the transformed Hamiltonian we set up a system of differential-equations for the single electronic and vibrational operators. For $\tilde{a}_1^+$ and $\tilde{a}_2^+$ we get

$$\frac{\partial}{\partial \lambda} \tilde{a}_1^+ = e^{-\lambda \hat{S}} [a_1^+, \hat{S}] e^{-\lambda \hat{S}} = A \tilde{a}_1^+ - B \tilde{a}_2^+ , \tag{8 a}$$

$$\frac{\partial}{\partial \lambda} \tilde{a}_2^+ = e^{-\lambda \hat{S}} [a_2^+, \hat{S}] e^{-\lambda \hat{S}} = B \tilde{a}_1^+ , \tag{8 b}$$

with the abbreviations

$$A = \sum_j \eta_j (b_j^+ - b_j) \tag{9 a}$$

and

$$B = \xi . \tag{9 b}$$

A and B commute with $\hat{S}$.

The combination of (8 a) and (8 b) gives a second order differential equation for each of the two operators:

$$\frac{\partial^2}{\partial \lambda^2} \tilde{a}_i^+ - A \frac{\partial}{\partial \lambda} \tilde{a}_i^+ + B^2 \tilde{a}_i^+ = 0 \quad (i = 1, 2) . \tag{10}$$

The formal solutions of these equations are given by ($i = 1, 2$)

$$\tilde{a}_i^+ = c_1^{(i)} \exp\left\{\frac{\lambda}{2} (A + \sqrt{A^2 - 4 B^2})\right\} + c_2^{(i)} \exp\left\{\frac{\lambda}{2} (A - \sqrt{A^2 - 4 B^2})\right\} . \tag{11}$$

$c_1^{(i)}$ and $c_2^{(i)}$ ($i = 1, 2$) are free parameters, which still must be determined. We do this by expanding and comparing (1) and (11) up to the first order in λ. After some elementary calculations we get the new transformed operators in the form:

$$\tilde{a}_1^+ = \left\{a_1^+ \left(\cosh \frac{\lambda}{2} \sqrt{A^2 - 4 B^2} + \frac{A}{\sqrt{A^2 - 4 B^2}} \sinh \frac{\lambda}{2} \sqrt{A^2 - 4 B^2}\right) - 2 a_2^+ \frac{B}{\sqrt{A^2 - 4 B^2}} \sinh \frac{\lambda}{2} \sqrt{A^2 - 4 B^2}\right\} \exp\left(\frac{\lambda}{2} A\right) \tag{12 a}$$

and

$$\tilde{a}_2^+ = \left\{a_2^+ \left(\cosh \frac{\lambda}{2} \sqrt{A^2 - 4 B^2} - \frac{A}{\sqrt{A^2 - 4 B^2}} \sinh \frac{\lambda}{2} \sqrt{A^2 - 4 B^2}\right) + 2 a_1^+ \frac{B}{\sqrt{A^2 - 4 B^2}} \sinh \frac{\lambda}{2} \sqrt{A^2 - 4 B^2}\right\} \exp\left(\frac{\lambda}{2} A\right) . \tag{12 b}$$

Similarly, the differential-equation for the phonon-operator b_j^+ reads

$$\frac{\partial}{\partial \lambda} \tilde{b}_j^+ = e^{-\lambda \hat{S}} [b_{j_1}^+ \hat{S}] e^{\lambda \hat{S}} = -\eta_j \tilde{a}_1^+ \tilde{a}_1 . \tag{13}$$

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* v ist a measure for the electron-electron coupling strength.

This equation can be easily integrated by inserting (12 a) into the right hand side. We get

$$\tilde{b}_j^+ = b_j^+ - \eta_j \left\{ \lambda\, a_1^+ a_1 + 2\,(a_1^+ a_1 - a_2^+ a_2) \left(\frac{B}{\sqrt{A^2-4\,B^2}} \right)^2 \left(\lambda - \frac{\sinh \lambda \sqrt{A^2-4\,B^2}}{\sqrt{A^2-4\,B^2}} \right) \right. \tag{14}$$
$$\left. + \, (a_1^+ a_2 - a_2^+ a_1)\, \frac{A\,B}{\sqrt{A^2-4\,B^2}^{\,2}} \left(\lambda - \frac{\sinh \lambda \sqrt{A^2-4\,B^2}}{\sqrt{A^2-4\,B^2}} \right) \right\}.$$

Now each operator appearing in the original Hamiltonian (5) is transformed, and we set $\lambda = 1$. The Hamiltonian in the new coordinates can be written down in a closed analytic form by inserting (12 a), (12 b), (14) and their hermitian conjugates into (5). However, in our results there are still free parameters, ξ and η_j. They can be chosen by putting the nondiagonal term of the Hamiltonian (or parts of it) equal to zero or by minimizing the energy by a variational procedure with respect to ξ and η_j.

Since in our case the transformed Hamiltonian is very lengthy and complicated, we will restrict our illustrative consideration to two simplified examples, which have been handled earlier in a different approach[4].

α) First, we set the electron-electron coupling parameter v equal zero ($v = 0$). Then it is obvious that ξ has to be zero too. This leads to transformed operators of the form

$$\tilde{a}_1^+ = a_1^+ \exp\{\sum_j \eta_j (b_j^+ - b_j)\} \tag{15 a}$$

$$\tilde{a}_2^+ = a_2^+ , \tag{15 b}$$

$$\tilde{b}_j^+ = b_j^+ - \eta_j\, a_1^+ a_1 , \tag{15 c}$$

and the Hamiltonian in the new space is given by

$$\tilde{H} = a_1^+ a_1 \{\varepsilon_1 + \sum_j \omega_j \eta_j^2 - 2 \sum_j K_j \eta_j\} + \varepsilon_2\, a_2^+ a_2 \tag{16}$$
$$+ \sum_j \omega_j\, b_j^+ b_j + a_1^+ a_1 \sum_j \{K_j - \omega_j \eta_j\} (b_j^+ + b_j) .$$

Choosing $\eta_j = K_j/\omega_j$ the non-diagonal part in (16) vanishes. The eigenvalues of the diagonalized Hamiltonian read

$$\tilde{\varepsilon}_1 = \varepsilon_1 - \sum_j K_j^2/\omega_j ; \quad \tilde{\varepsilon}_2 = \varepsilon_2 . \tag{17}$$

β) Second, we assume the electron-phonon coupling to be zero ($K_j = 0$). Then η_j follows to be also zero ($\eta_j = 0$; $A = 0$). From (12 a) and (12 b) we get the equations

$$\tilde{a}_1^+ = a_1^+ \cos \xi + a_2^+ \sin \xi , \tag{18 a}$$

$$\tilde{a}_2^+ = -\, a_1^+ \sin \xi + a_2^+ \cos \xi . \tag{18 b}$$

The transformed Hamiltonian takes the form

$$\tilde{H} = \left\{ \frac{\varepsilon_1+\varepsilon_2}{2} + \frac{\varepsilon_1-\varepsilon_2}{2} \cos 2\,\xi + v \sin 2\,\xi \right\} a_1^+ a_1 \tag{19}$$
$$+ \left\{ \frac{\varepsilon_1+\varepsilon_2}{2} - \frac{\varepsilon_1-\varepsilon_2}{2} \cos 2\,\xi - v \sin 2\,\xi \right\} a_2^+ a_2$$
$$+ \left\{ v \cos 2\,\xi - \frac{\varepsilon_1-\varepsilon_2}{2} \sin 2\,\xi \right\} (a_1^+ a_2 + a_2^+ a_1) .$$

We choose the free parameter ξ in such a form that the non-diagonal part of the Hamiltonian vanishes. After some transcriptions one gets

$$\sin 2\,\xi = \frac{2\,v}{\sqrt{(\varepsilon_1-\varepsilon_2)^2 + 4\,v^2}} ; \tag{20}$$
$$\cos 2\,\xi = \frac{(\varepsilon_1-\varepsilon_2)}{\sqrt{(\varepsilon_1-\varepsilon_2)^2 + 4\,v^2}}$$

and from this

$$\xi = \frac{1}{2} \arc\tan \frac{2\,v}{(\varepsilon_1-\varepsilon_2)} .$$

Then the eigenvalues of the transformed and exactly diagonalized Hamiltonian are given by

$$\tilde{\varepsilon}_{1/2} = \tfrac{1}{2} \{ (\varepsilon_1+\varepsilon_2) \pm \sqrt{(\varepsilon_1-\varepsilon_2)^2 + 4\,v^2} \} . \tag{22}$$

4. The Zero Phonon Line of the Optical Absorption Spectrum

In this section we are specifically interested in the optical response of the combined systems to an electromagnetic stimulus from outside, which interacts only with the electronic subsystem. Under the influence of the electromagnetic lightfield, which may be polarized in such a form that it affects only centre No. 1, an optical transition is made from the initial state $\overline{\psi}^{\mathrm{I}}(x, q)$ to the final state $\overline{\psi}^{\mathrm{F}}(x, q)$. Then the dipol operator is given by

$$P^{(1)}(x) = e\, x_1 = p\,(a_1^+ + a_1) . \tag{23}$$

Furtheron, if we confine us to $T = 0\ {}^\circ\mathrm{K}$, only the absolute ground state $|0\rangle$ contributes to be the initial state. Under these assumptions the optical absorption function reaches the form[6]

$$G(\omega) = \sum_m |\langle \overline{\psi}_m^{\mathrm{F}}(x, q) |\, a_1^+ + a_1 \,| 0 \rangle|^2\, \delta(E_m^{\mathrm{F}} - \omega) . \tag{24}$$

ω is the energy of the external lightfield. The index m denotes the number of phonons, which accompany to the excited electronic state, and E_m^F is the energy of this vibronic state. It is given in Ref. [1] [Eq. (20 a)] and can be calculated by the procedure given in the previous section. But this value is of no importance in our context. If we confine ourselves to the calculation of the zero phonon line, the sum over m [in (24)] is reduced to the single term with $m = 0$.

In the previous section we have transformed the system to a new basis. By a suitable choice of the parameters ξ and η_j the new Hamiltonian is diagonal or at least nearly diagonal. Then the eigenfunctions are product functions, e. g.

$$\tilde{\psi}_0^F(x, q) = a_i^+ | 0\rangle \quad (i = 1, 2) . \tag{25}$$

With $\exp[\hat{S}] | 0\rangle = | 0\rangle$ we get for the zero phonon line

$$G_0(\omega) = | \langle \tilde{\psi}_0^F(x, q) | e^{-\hat{S}} | a_1^+ 0\rangle |^2 \, \delta(E_0^F - \omega) . \tag{26}$$

A direct electronic transition from the ground state to the excited state $a_2^+ | 0\rangle$ is forbidden (see Reference [3]). The remaining matrix element which we have to calculate reads

$$\begin{aligned} \langle 0\, a_1^+ | e^{-\hat{S}} | a_1^+ 0\rangle &= \sum_{n=0}^{\infty} \frac{(-1)^n}{n!} \langle 0\, a_1^+ | \{ -\xi (a_1^+ a_2 - a_2^+ a_1) \\ &\quad - a_1^+ a_1 \sum_j \eta_j (b_j^+ - b_j) \}^n | a_1^+ 0\rangle . \end{aligned} \tag{27}$$

The integration over the electronic coordinates can be done by combinatorial analysis. It is given in Appendix A. For Eq. (27) we get

$$\begin{aligned} \sum_{n=0}^{\infty} \frac{1}{(2n)!} \sum_{\alpha=0}^{n} \binom{n+\alpha}{2\alpha} (-1)^{n-\alpha} \xi^{2(n-\alpha)} \\ \langle 0 | \{ \sum_j \eta_j (b_j^+ - b_j) \}^{2\alpha} | 0\rangle , \end{aligned} \tag{28}$$

and after solving the matrix elements over the phonon coordinates (see Ref. [6]):

$$\sum_{n=0}^{\infty} \frac{(-1)^n}{(2n)!} \xi^{2n} \sum_{\alpha=0}^{n} \binom{n+\alpha}{2\alpha} \frac{(2\alpha)!}{\alpha!} \left\{ \frac{\sum_j \eta_j^2}{2\xi^2} \right\}^{\alpha} . \tag{29}$$

Introducing the function $K_{n+1/2}(Z)$ which belongs to the family of Bessel functions [7],

$$\begin{aligned} K_{n+1/2}(Z) &= \sqrt{\frac{\pi}{2Z}}\, e^{-Z} \sum_{\alpha=0}^{n} \frac{(n+\alpha)!}{\alpha!\,(n-\alpha)!} \left(\frac{1}{2Z}\right)^{\alpha} \\ &= \int_0^{\infty} e^{-Z \cosh t} \cosh[(n+\tfrac{1}{2}) t]\, dt , \end{aligned} \tag{30}$$

the matrix element (29) can be written in the form

$$\langle 0\, a_1^+ | e^{-\hat{S}} | a_1^+ 0\rangle = \sum_{n=0}^{\infty} \frac{(-1)^n}{(2n)!} \xi^{2n} \sqrt{\frac{2Z}{\pi}}\, e^{Z} K_{n+1/2}(Z) \tag{31}$$

with

$$Z = \xi^2 / \sum_j \eta_j^2 . \tag{32}$$

The integral representation of $K_{n+1/2}(Z)$ [Eq. (30)] allows a further simplification of Expr. (31), and after some elementary transcriptions one gets the final result

$$I_0 = \langle 0\, a_1^+ | e^{-\hat{S}} | a_1^+ 0\rangle = \int_0^{\infty} \exp\left[-\frac{Z}{2} \left(u^2 + \frac{1}{u^2} \right) \right] \cos(\xi u)\, du \tag{33}$$

and for the zero phonon line

$$G_0 = I_0^2 . \tag{34}$$

G_0 is drawn in Figs. 1 a and 1 b in dependence of Z. For all values of Z G_0 is finite. In Fig. 1 a the electron-electron coupling ξ is constant and the electron-phonon coupling $\sqrt{\sum \eta_j^2}$ is varied. In Fig. 1 b $\sqrt{\sum \eta_j^2}$ is constant and ξ is varied. From the figures we see that the function G_0 reflects the resonant nature of the system.

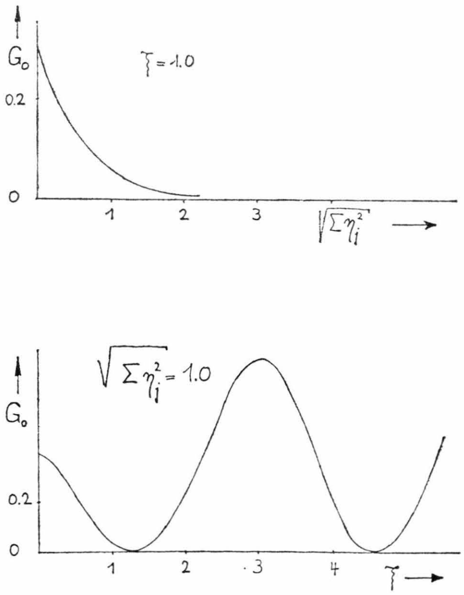

Fig. 1. Intensity of the zero phonon line in dependence of the coupling parameters. a) The parameter ξ, which is related to the electron-electron coupling is 1.0. The parameter $\sqrt{\sum \eta^2}$, which is related to the electron phonon coupling is varied. b) The parameter $\sqrt{\sum \eta^2}$ is 1.0. The parameter ξ is varied. (Explanation see text.)

In the extremal coupling regions G_0 can be written in very simplified forms. For $Z \to 0$ ($\xi^2 \to 0$, $\Sigma \eta^2 = \text{const}$, or $\Sigma \eta^2 \to \infty$, $\xi^2 = \text{const}$) one gets

$$G_0 = \exp\{-\sum_j \eta_j^2\}, \tag{35}$$

and for $Z \to \infty$ ($\xi^2 \to \infty$, $\Sigma \eta^2 = \text{const}$, or $\Sigma \eta^2 \to 0$, $\xi^2 = \text{const}$)

$$G_0 = \cos^2 \xi. \tag{36}$$

In Figs. 1 a and 1 b this limiting behaviour can be seen.

5. Summary and Discussion

Usually the treatment of canonical exponential transformations in a closed analytic form is very cumbersome. In this article we have derived a method which is very useful for practical calculations. The problem of summing up a commutator series expansion is transferred to the treatment of a system of coupled differential equations.

The derived method allows the transformation of each single operator in a closed analytic form. However, in many cases the system of differential-equations will be very complicated and the decoupling procedure rather cumbersome. In such situations the differential-equations can be solved approximatively. This can be done by neglecting small terms in the equations or by a decoupling procedure of the hierarchy, in the sense of the factorization decoupling by the Green's function technique. The transformed quantities then again are given in closed forms. In most of the cases the results are more accurate than usual perturbative results, and they allow the analytic description of resonance effects.

For an illustration of the method an antiresonant electron-phonon system (Fano system) is calculated. The single system operators are transcribed by a general transformation exhibiting two free parameters. In two different limiting cases the transformed Hamiltonian is given.

Furtheron, the zero phonon line of the optical absorption spectrum is calculated for arbitrary coupling strengths. It shows a resonant behaviour as one would expect by systems of such a nature. Especially it is to be seen that the intensity of the zero phonon line has totally different structures if one or the other of the coupling parameters is varied (Fig. 1 a and Figure 1 b). As will be shown in the near future, this effect manifest itself also in the whole absorption spectrum and indicates a change (in the sense of a phase transition) of the internal subdynamics of the system.

Appendix A

In accordance to the calculations of Wagner [8] for the E–e J.T. system and of the author [9] for the T–t J.T. system the integration over the electronic coordinates can be done by combinatorial analysis:

$$\langle 0\, a_1^+ | \{ -\xi (a_1^+ a_2 - a_2^+ a_1) - a_1^+ a_1 \sum_j \eta_j (b_j^+ - b_j) \}^n | a_1^+\, 0 \rangle . \tag{A.1}$$

The calculation leads to a combinatorial problem, which may be depicted in a diagram. In Fig. 2 all elements of a general diagram are drawn. Only these combinations of operators give nonvanishing terms, in which the attached arrows form closed paths, beginning and ending on line 1. In Fig. 2 one possible path is drawn. α, β, γ are the numbers, how often the different elements appear in each single product term in Expression (A.1). The following relations must be satisfied:

$$\alpha + \beta + \gamma = n, \quad \beta = \gamma, \quad \alpha + 2\gamma = n. \tag{A.2}$$

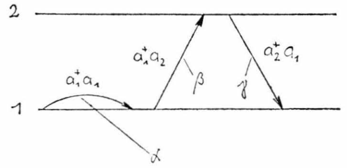

Fig. 2. All possible elements arising by the integration in the electronic subsystem, characterized by different arrows. α, β and γ count the number of appearence of the different elements in the operator product.

From the diagram of Fig. 2 it is easy to see that the terms $a_1^+ a_1$ can be located onto $(\gamma + 1)$ different places. This leads us to the question: What is the number of distinguishable arrangements of α indistinguishable objects in $(\gamma + 1)$ distinct cells (places), where any cell may contain 0, 1, 2, . . . or α objects? The answer is well-known from combinatorial analysis [8]

$$Z(\alpha, \gamma) = \binom{\gamma + \alpha}{\alpha} = \binom{\gamma + \alpha}{\gamma}. \tag{A.3}$$

If we insert (A.2) into (A.3) and distinguish between $n = \text{even}$ ($\sim > \alpha = \text{even}$) and $n = \text{odd}$ ($\sim > \alpha = \text{odd}$) we get for (A.1)

$$\sum_{n=0}^{n} \binom{n+\alpha}{2\,\alpha} (-1)^{n-\alpha}\, \xi^{2(n-\alpha)} \langle 0 | \{\textstyle\sum \eta_j (b_j^+ - b_j)\}^{2\alpha} | 0 \rangle \,. \tag{A.4}$$

The term with $n = \text{odd}$ vanishes, because of the integration over the phonon coordinates.

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