

# Derivation of Phonon Assisted Auger Transition Probabilities in Semiconductors

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In this paper a theory developed by Stumpf [1] will be used in order to calculate Auger transition probabilities in semiconductors. The main feature of the calculations is the incorporation of the coupling of impurity electrons to the surrounding lattice by phonons, using dynamical electronic wave functions for impurity states. The final result is an expression for transition probabilities, describing multiphonon assisted Auger transitions in semiconductors.

## Introduction

The optical properties of impurity centers in semiconductors are often described in a one-impurity center approximation. In this model all processes at one center are independent of the presence of other surrounding impurities. For large concentrations of defects this assumption cannot be justified any longer and interactions between centers have to be taken into account. A particularly interesting case of interaction is the resonant transfer of excitation energy from one impurity to another. There are two mechanisms leading to such processes, first the reabsorption of radiation emitted by decaying excited centers, and secondly the direct Coulomb and exchange interaction between these centers. The latter processes are called Auger transitions. In this paper we will discuss these processes. Our model is based on a theory developed by Stumpf and coworkers [1–7]. In this theory in a first step a microblock model is proposed to describe processes at one impurity center. In a second step these microblocks are collected to form a mosaicblock which will be the basic model for our calculations.

Auger processes in semiconductors were often studied in literature. There are many papers by Landsberg and coworkers [8–12]. They try to calculate Auger recombination rates and impact ionisation coefficients. In their calculations Landsberg et al. restrict themselves to the pure electronic part of the transitions without coupling to the phonons. This restriction may be justified for semiconductors with narrow energy gaps or impurities with low trap depth. Similar calculations were made

by Haug [13, 14] and Schöne [15] for band-band transitions.

On the other side, there are only few investigations about the phonon assisted transitions. Eagles [16] used the second order perturbation theory to include phonons in the transitions via the electron phonon interaction. Another method of Rosenthal [17] provides a unitary transformation of the perturbation part of the Hamiltonian, consisting of an electron-electron and an electron-phonon interaction part, to describe such processes. By this way Auger transition probabilities for creation or destruction of two phonons are obtained.

In this paper we investigate by means of the theory mentioned above the transition probabilities with an arbitrary number of phonons. Thereby we restrict ourselves to pure theoretical discussions without numerical results which will be given in a following paper. In the first section we summarize all the definitions we need. In section 2 the basic theory for our calculations will be outlined. In a further section we calculate the Auger operator for the special case of halogenid crystals with colour centers. Then we treat in the following section the corresponding Auger transition probabilities and derive calculable expressions.

## 1. Definitions

All abbreviations to be used are given in this first section. If possible, the notations of paper [1] are applied.

### a) Notation of the Crystal Structure

- $e$  := charge of the electron;
- $r_i$  := position of the  $i$ -th impurity electron;
- $l$  := index of the  $l$ -th elementary cell of the ideal lattice;

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- $\mu$  := index of the ions in the elementary cell;  
 $e_{l\mu}$  := charge of the  $l\mu$ -th nucleus;  
 $\mathfrak{R}_{l\mu}^0$  := ideal lattice position of the  $l\mu$ -th nucleus;  
 $\mathfrak{R}_{l\mu}$  := lattice position of the  $l\mu$ -th nucleus in the distorted lattice;  
 $\mathfrak{R}_{l\mu}^n$  := static lattice position of the  $l\mu$ -th nucleus in the distorted lattice when the impurity electron is in state  $n$ ;  
 $a_{l\mu} := (e_{l\mu} + \sum_{\alpha_{l\mu}} e)$  charge of the  $l\mu$ -th ion; (1.1)  
 $\mathfrak{M}_{l\mu} := \mathfrak{R}_{l\mu} - \mathfrak{R}_{l\mu}^0$ , ionic displacement from ideal lattice position; (1.2)  
 $X_{l\mu}^n := \mathfrak{R}_{l\mu} - \mathfrak{R}_{l\mu}^n$ , ionic displacement from static lattice position when the impurity electron is in state  $n$ ; (1.3)  
 $l^i \mu^i$  with  $1 \leq i \leq s$  := lattice points of the impurities; (1.4)  
 $\sum_{(l\mu)}$  := sum over all lattice points excluding  $l^i \mu^i$ ,  $1 \leq i \leq s$ ; (1.5)  
 $\sum_{i,j}$  :=  $\sum_{i,j}$  with  $i \neq j$ ; (1.6)  
 $C(\mathbf{r}, \mathbf{r}') := |\mathbf{r} - \mathbf{r}'|^{-1}$ ,  
 $C(\mathbf{r}, \mathfrak{R}_{l\mu}) := |\mathbf{r} - \mathfrak{R}_{l\mu}|^{-1}$ , (1.7)  
 $C(\mathbf{r}, l\mu) := |\mathbf{r} - \mathfrak{R}_{l\mu}^0|^{-1}$ , Coulomb potentials;  
 $m$  := electron mass; (1.8)  
 $M_{l\mu}$  := mass of the  $l\mu$ -th nucleus. (1.9)
- $\eta, \kappa \in \mathbb{M} := \{\varrho_\varepsilon | \varrho = l^i \mu^i \text{ resp. } c \text{ with } 1 \leq i \leq s \text{ and } \varepsilon = 1, \dots, r, k\}$   
 := quantum number of impurity states; (1.18)  
 $\psi_\eta(\mathbf{r}, \mathfrak{R})$  := one particle functions of the impurity state; (1.19)  
 $a_{\alpha_{l\mu}}^n(\mathbf{r}, \mathfrak{R})$  := one particle functions of the atomic state  $\alpha$  in the  $l\mu$ -th ion; (1.20)  
 $m_{l\mu}^n := \sum_{\alpha_{l\mu}} e \int a_{\alpha_{l\mu}}^{n*} a_{\alpha_{l\mu}}^n (\mathbf{r} - \mathfrak{R}_{l\mu}) d\mathbf{r}$   
 := electronic dipole moment of the  $l\mu$ -th ion; (1.21)  
 $q_t^n := \sum_{(l\mu)} B_{t,l\mu}^n X_{l\mu}^n$ : normal coordinates of the mosaicblock crystal; (1.22)  
 $\beta^n(X^n)$  := variational parameters of the dynamic electronic wave functions as function of the displacements  $X_{l\mu}^n$ ; (1.23)  
 $a_t^{nn'}$  := normal coordinate displacements for an electronic transition from  $n'$  to  $n$ ; (1.24)  
 $\gamma_m^n(E_m^n)$  := line width of phonon state  $m$  with energy value  $E_m^n$ ; (1.25)  
 $E_m^n$  := energy value of the mosaicblock crystal; (1.26)  
 $\overline{E}_m^n$  := energy value of the mosaicblock crystal in harmonic approximation; (1.27)

#### b) Quantum Mechanical and Thermodynamic Quantities

- $\beta := (kT)^{-1}$  Boltzmann factor; (1.10)  
 $Z_{\text{Phon}}$  := partition function of the whole phonon system; (1.11)  
 $f_m(T) := Z_{\text{Ph}}^{-1} \exp\{-\beta E_m^n\}$  thermo-dynamic steady state distribution of the phonon system; (1.12)  
 $p_\nu(t)$  := occupation probability of the  $\nu$ -th photon mode; (1.13)  
 $\hat{Q}(t)$  := statistical operator of the whole mosaicblock system; (1.14)  
 $\chi_n^c(\mathbf{r}, \mathfrak{R})$  := total electronic wave function; (1.15)  
 $q_m^n(\mathfrak{R})$  := total lattice wave function of the mosaicblock; (1.16)  
 $\alpha_{l\mu}$  := shell quantum number of the  $l\mu$ -th ion; (1.17)

#### c) Calculation Aids for Phonon Assisted Auger Transitions

- $\Delta_{\eta\kappa, \eta'\kappa'} := (1 - \delta_{\eta\kappa, \eta'\kappa'} \delta_{m, m'})$ ; (1.28)  
 $\varrho_t, \bar{\varrho}_t, \varrho_t', \bar{\varrho}_t', \varrho_t^*, \bar{\varrho}_t^*, \varrho_t'^*, \bar{\varrho}_t'^*, \gamma_t, \bar{\gamma}_t, \gamma_t^*, \bar{\gamma}_t^* \equiv$  parameters;  
 $p_t^\eta := \sqrt{\hbar \omega_t^\eta / 2} (a_t^{\eta+} - a_t^\eta)$ ; (1.29)  
 $a_t^{\eta+}, a_t^\eta$  := oscillator creation and destruction operators of frequency  $\omega_t^\eta$ ; (1.30)  
 $\hat{U}_t^\eta := \exp\{i p_t^\eta a_t^{\eta+}\}$ ; (1.31)  
 $A_t^\eta := \frac{\omega_t^\eta - \omega_t^{\eta'}}{2(\omega_t^\eta + \omega_t^{\eta'})}$ ; (1.32)  
 $B_t^\eta := \frac{\omega_t^{\eta 2} - \omega_t^{\eta' 2}}{8\omega_t^\eta \omega_t^{\eta'}}$ ; (1.33)  
 $\hat{V}_t^\eta := \exp\{-A_t^\eta (a_t^\eta)^2\} \exp\{B_t^\eta (a_t^{\eta+})^2\}$ ; (1.34)  
 $c_{m_t}^\eta := \langle \Phi_{m_t}^\eta | \hat{V}_t^{\eta+} \hat{V}_t^\eta | \Phi_{m_t}^\eta \rangle$ ; (1.35)  
 $\alpha_t^{\eta\eta'} := \sqrt{2\omega_t^\eta / \hbar} a_t^{\eta\eta'}$ ; (1.36)

$$d_{1,t}^{\eta\eta'(*)} := -\alpha_t^{\eta\eta'} + \sqrt{\hbar/2\omega_t^{\eta}} \gamma_t^{(*)}; \quad (1.37)$$

$$d_{2,t}^{\eta\eta'(*)} := \alpha_t^{\eta\eta'} + \sqrt{\hbar/2\omega_t^{\eta}} \gamma_t^{(*)}; \quad (1.38)$$

$$d_{3,t}^{\eta\eta'(*)} := \frac{\hbar}{2\omega_t^{\eta}} \gamma_t^{(*)2} - (\alpha_t^{\eta\eta'})^2 - 2 \sqrt{\frac{\hbar}{2\omega_t^{\eta}}} \alpha_t^{\eta\eta'} \gamma_t^{(*)}; \quad (1.39)$$

$$f_{0,t}^{\eta\eta'} := \frac{A_t^{\eta} - B_t^{\eta}}{(1 - \exp\{-\beta \hbar \omega_t^{\eta}\})^2} \cdot (d_{2,t}^{\eta\eta'} d_{2,t}^{\eta\eta'*} - d_{1,t}^{\eta\eta'} d_{1,t}^{\eta\eta'*} \exp\{-\beta \hbar \omega_t^{\eta}\}); \quad (1.40)$$

$$f_{1,t}^{\eta\eta'} := \frac{A_t^{\eta} + B_t^{\eta}}{(1 - \exp\{-\beta \hbar \omega_t^{\eta}\})^2} \cdot (d_{1,t}^{\eta\eta'} d_{2,t}^{\eta\eta'} + d_{1,t}^{\eta\eta'*} d_{2,t}^{\eta\eta'*}) \exp\{-\beta \hbar \omega_t^{\eta}\}; \quad (1.41)$$

$$f_{2,t}^{\eta\eta'} := \frac{A_t^{\eta} + B_t^{\eta}}{(1 - \exp\{-\beta \hbar \omega_t^{\eta}\})^2} \cdot d_{1,t}^{\eta\eta'} d_{1,t}^{\eta\eta'*} \exp\{-2\beta \hbar \omega_t^{\eta}\}; \quad (1.42)$$

$$f_{3,t}^{\eta\eta'} := -\frac{A_t^{\eta} + B_t^{\eta}}{(1 - \exp\{-\beta \hbar \omega_t^{\eta}\})^2} d_{2,t}^{\eta\eta'} d_{2,t}^{\eta\eta'*}; \quad (1.43)$$

$$c_t^{\eta\eta'} := \frac{1}{1 - \exp\{-\beta \hbar \omega_t^{\eta}\}} d_{2,t}^{\eta\eta'} d_{2,t}^{\eta\eta'*}; \quad (1.44)$$

$$b_t^{\eta\eta'} := \frac{\exp\{-\beta \hbar \omega_t^{\eta}\}}{1 - \exp\{-\beta \hbar \omega_t^{\eta}\}} d_{1,t}^{\eta\eta'} d_{1,t}^{\eta\eta'*}; \quad (1.45)$$

$$g_{\nu_t}^{\eta\eta'} := \sum_{n_1, \dots, n_4} \frac{(f_{1,t}^{\eta\eta'})^{n_1}}{n_1!} \frac{(-f_{1,t}^{\eta\eta'})^{n_2}}{n_2!} \cdot \frac{(f_{2,t}^{\eta\eta'})^{n_3}}{n_3!} \frac{(f_{3,t}^{\eta\eta'})^{n_4}}{n_4!} \delta_{\nu_t, n_1 - n_2 + 2n_3 - 2n_4}. \quad (1.46)$$

## 2. Basic Theory

To describe Auger transitions in semiconductors with point defects we use the mosaicblock model introduced by Stumpf [4] as our basic concept of deduction. We write the Hamiltonian for this model as:

$$\hat{H} := \hat{K} + \hat{S} + \hat{W} + \hat{H}^s + \hat{H}^w \quad (2.1)$$

with:

- $\hat{K}$  energy operator of the whole mosaic block,
- $\hat{S}$  operator of the free radiation field,
- $\hat{W}$  operator of the heat bath,
- $\hat{H}^s$  interaction operator between crystal and radiation field,
- $\hat{H}^w$  interaction operator between the surrounding heat bath and mosaicblock crystal.

This mosaicblock system is described by the base states:

$$|a\rangle \equiv |n m \nu \varrho\rangle := |n m\rangle \otimes |\nu\rangle \otimes |\varrho\rangle, \quad (2.2)$$

where the subsystems are represented as follows:

- $|n m\rangle$  the dynamic electron lattice states of the crystal with electronic quantum number  $n$  and lattice quantum number  $m$ ,
- $|\nu\rangle$  the eigenstates of the radiation field and
- $|\varrho\rangle$  the states of the coupled heat bath.

As a further step we represent the electron lattice states in the adiabatic coupling scheme [18]. They are given in the coordinate representation with the definitions (1.15) and (1.16) by:

$$\begin{aligned} \langle \mathfrak{r}, \mathfrak{R} | n m \rangle &\equiv \chi_n^c(\mathfrak{r}, \mathfrak{R}) \varphi_m^n(\mathfrak{R}) \\ &=: |\chi_n^c\rangle |\varphi_m^n\rangle. \end{aligned} \quad (2.3)$$

The states (2.2) and (2.3) are not eigenstates of the Hamiltonian (2.1). Therefore we have developed a method to define all perturbations of the system which cause transitions between these base states. Among these transitions we shall also find Auger transitions. To derive them let us define the crystal-Hamiltonian as

$$\hat{K} := \sum_{\{l\mu\}} (-\hbar^2/2M_{l\mu}) \Delta_{\mathfrak{R}_{l\mu}} + \hat{h}(\mathfrak{R}, \mathfrak{r}), \quad (2.4)$$

where in  $\hat{h}(\mathfrak{R}, \mathfrak{r})$  the kinetic energy of the electrons and all Coulomb interactions of charged particles being in the crystal are collected. The solution of the equations

$$\hat{h}(\mathfrak{R}, \mathfrak{r}) |\chi_n^c\rangle = \tilde{U}_n(\mathfrak{R}) |\chi_n^c\rangle, \quad (2.5)$$

$$\left[ \sum_{\{l\mu\}} -\frac{\hbar^2}{2M_{l\mu}} \Delta_{\mathfrak{R}_{l\mu}} + \tilde{U}_n(\mathfrak{R}) \right] |\varphi_m^n\rangle = \tilde{E}_m^n |\varphi_m^n\rangle \quad (2.6)$$

leads to the adiabatic states (2.3) and a perturbation operator  $\hat{K}^t$  which will be defined later.

The electronic equation (2.5) will be treated by means of the Hartree-Fock variational principle which gives also no exact eigenstates and eigenvalues. Consequently, we get the approximative expression for the eigenvalue

$$U_n(\mathfrak{R}) := \text{Min}_{\{|\chi_n^c\rangle\}} \langle \chi_n^c | \hat{h}(\mathfrak{R}, \mathfrak{r}) | \chi_n^c \rangle \quad (2.7)$$

and a nondiagonal part  $\hat{k}^s$  in (2.5) remains. The Eqs. (2.5) and (2.6) then read:

$$\hat{h}(\mathfrak{R}, \mathfrak{r}) |\chi_n^c\rangle = [U_n(\mathfrak{R}) \mathbf{1} + \hat{k}^s(\mathfrak{R})] |\chi_n^c\rangle, \quad (2.5a)$$

$$\left[ \sum_{\{\mu\}} -\frac{\hbar^2}{2M_{l\mu}} \Delta_{\mathfrak{R}_{l\mu}} + U_n(\mathfrak{R}) \right] |\varphi_m^n\rangle = E_m^n |\varphi_m^n\rangle. \quad (2.6a)$$

The result of these considerations is finally a separation of the Hamiltonian (2.1) in two parts:

$$\hat{H} = \hat{H}_0 + \hat{H}_1, \quad (2.8)$$

where  $\hat{H}_0$  represents the diagonal part between the states (2.2) of  $\hat{H}$  and is given by

$$\hat{H}_0 := \sum_{nm\nu q} |n m \nu q\rangle \langle n m \nu q| \hat{H} |n m \nu q\rangle \langle n m \nu q| \quad (2.9)$$

while the nondiagonal perturbation operator  $\hat{H}_1$  can be worked out to be

$$\hat{H}_1 := \hat{H} - \hat{H}_0 = \hat{K}^t + \hat{K}^s + \hat{H}^s + \hat{H}^w. \quad (2.10)$$

The various operators in this definition are represented by the following matrix elements:

$$\begin{aligned} K_{n'm'\nu'q'}^{nm\nu q} &:= (1 - \delta_{nn'} \delta_{mm'}) \delta_{\nu\nu'} \delta_{qq'} \\ &\cdot \sum_{\{\mu\}} -\frac{\hbar^2}{2M_{l\mu}} [\langle \chi_n^c | \Delta_{\mathfrak{R}_{l\mu}} | \chi_{n'}^c \rangle \langle \varphi_m^n | \varphi_{m'}^{n'} \rangle \\ &+ 2 \langle \chi_n^c | \nabla_{\mathfrak{R}_{l\mu}} | \chi_{n'}^c \rangle \langle \varphi_m^n | \nabla_{\mathfrak{R}_{l\mu}} | \varphi_{m'}^{n'} \rangle], \end{aligned} \quad (2.11)$$

$$\begin{aligned} K_{n'm'\nu'q'}^{s, nm\nu q} &:= (1 - \delta_{nn'} \delta_{mm'}) \delta_{\nu\nu'} \delta_{qq'} \\ &\cdot \langle \varphi_m^n \chi_n^c | \hat{h}(\mathfrak{R}, \mathbf{r}) | \chi_{n'}^c \varphi_{m'}^{n'} \rangle \\ &= (1 - \delta_{nn'} \delta_{mm'}) \delta_{\nu\nu'} \delta_{qq'} \\ &\cdot \langle \varphi_m^n | \hat{k}^s | \varphi_{m'}^{n'} \rangle. \end{aligned} \quad (2.12)$$

with

$$\hat{k}^s(\mathfrak{R}) := \langle \chi_n^c | \hat{h}(\mathfrak{R}, \mathbf{r}) | \chi_{n'}^c \rangle; \quad (2.13)$$

$$\begin{aligned} H_{n'm'\nu'q'}^{s, nm\nu q} &:= (1 - \delta_{nn'} \delta_{mm'}) \delta_{\nu\nu'} \delta_{qq'} \\ &\cdot \langle \chi_n^c \varphi_m^n \nu | \hat{H}^s | \nu' \varphi_{m'}^{n'} \chi_{n'}^c \rangle; \end{aligned} \quad (2.14)$$

$$\begin{aligned} H_{n'm'\nu'q'}^{w, nm\nu q} &:= (1 - \delta_{mm'}) \delta_{qq'} \delta_{\nu\nu'} \delta_{nn'} \\ &\cdot \langle \varphi_m^n q | \hat{H}^w | q' \varphi_{m'}^{n'} \rangle. \end{aligned} \quad (2.15)$$

The effects of these interactions can be classified as follows:

- $\hat{K}^t$ : is a nonadiabatic interaction which produces multiphonon transitions,
- $\hat{K}^s$ : is a Coulomb interaction between impurity electrons alone or between impurity electrons and surrounding ions and leads especially to Auger transitions,
- $\hat{H}^s, \hat{H}^w$ : represent the interaction between radiation field and the heat bath with the

crystal respectively and cause radiative electron and/or phonon processes and energy dissipative processes of the highly excited phonons.

To describe the behaviour of the whole mosaic-block system with its various interactions, we consider the occupation possibilities:

$$P_{nm\nu q} := \text{Sp}[\hat{\rho}(t) \mathbb{P}_{nm\nu q}] \quad (2.16)$$

with the projector

$$\mathbb{P}_{nm\nu q} := |n m \nu q\rangle \langle n m \nu q|. \quad (2.17)$$

The time dependent behaviour of these probabilities is governed by the Pauli Master equation [1–3]:

$$P_{nm\nu q}(t) = \sum_{n'm'\nu'q'} W_{n'm'\nu'q'}^{nm\nu q} [P_{n'm'\nu'q'}(t) - P_{nm\nu q}(t)]. \quad (2.18)$$

Thereby the differential transition probabilities  $W_{n'm'\nu'q'}^{nm\nu q}$  are given with (2.10) in the first order perturbation approximation and in thermodynamic times by

$$\begin{aligned} W_{n'm'\nu'q'}^{nm\nu q} &:= (2\pi/\hbar) |\langle n m \nu q | \hat{H}_1 | n' m' \nu' q' \rangle|^2 \\ &\cdot \delta(E_m^n + E_\nu + E_q - E_{m'}^{n'} - E_{\nu'} - E_{q'}). \end{aligned} \quad (2.19)$$

In the dynamical equation (2.18) all degrees of freedom of the different subsystems are contained. If we are only interested in the electronic reactions, all other degrees of freedom must be eliminated. This was done by Stumpf and coworkers [1, 2, 4, 19], resulting in the equation:

$$\begin{aligned} p_n(t) &= \sum_{n'} [W_{nn'}^k(T) + W_{nn'}^s(T, t)] p_{n'}(t) \\ &- \sum_{n'} [W_{n'n}^k(T) + W_{n'n}^s(T, t)] p_n(t). \end{aligned} \quad (2.20)$$

The expressions in (2.20) are defined by means of the definitions (1.10), (1.11) and by the additional definitions

$$p_n(t) \text{ occupation probability of the electronic state } |\chi_n^c\rangle, \quad (2.21)$$

$$W_{nn'}^k(T) := \sum_{nm'} W_{mn, m'n'}^k f_{m'}(T) \text{ total non-radiative transition probabilities,} \quad (2.22)$$

$$W_{nn'}^s(T, t) := \sum_{\nu\nu'} \sum_{mm'} W_{nm\nu, n'm'\nu'}^s f_{m'}(T) p_{\nu'}(t) \text{ the total radiative transition probabilities.} \quad (2.23)$$

Thereby, in  $W_{nm, n'm'}^k$  and in  $W_{nm\nu, n'm'\nu'}^s$  are collected all nonradiative and all radiative transitions of the perturbation (2.10) respectively.



The Eqs. (2.20) for the electrons are the basic equations for the derivation of rate equations for any special model. This will be done for Auger reactions in a subsequent paper. In this paper we restrict ourselves to the definition (2.22) with the perturbation operator (3.12). Our aim is to derive multiphonon transition probabilities for Auger processes.

### 3. Auger Transitions for Colour Centers

In this section we derive explicitly the operator of Auger transitions (2.12) for a special model of ionic crystals with  $F$ - and  $F'$ -centers. We assume to have an idealized mosaicblock with  $s$  impurities in the above mentioned model. These impurities are  $F$ -,  $F'$ - and  $\alpha$ -centers. For the regular lattice points we assume  $M$  monovalent ions at the places  $\mathfrak{R}_{l\mu}$ . The impurities are localized at  $\mathfrak{R}_{l\mu'}$  (1.4). We assume that together with the  $N$  regular ion electrons there are  $s$  impurity electrons in the crystal.

The Hamiltonian of all charged particles within the mosaicblock reads

$$\hat{h}(\mathfrak{R}, \mathbf{r}) := \hat{h}_1(\mathfrak{R}, \mathbf{r}) + \hat{h}_2(\mathbf{r}) + \hat{V}(\mathfrak{R}) \quad (3.1)$$

with

$$\hat{h}_1(\mathfrak{R}, \mathbf{r}) := \sum_{i=1}^{N+s} \left( -\frac{\hbar^2}{2m} \Delta_{\mathbf{r}_i} + \sum_{\{l\mu\}} e e_{l\mu} C(\mathbf{r}_i, \mathfrak{R}_{l\mu}) \right), \quad (3.2)$$

$$\hat{h}_2(\mathbf{r}) := \frac{1}{2} \sum_{i,j=1}^{N+s} e^2 C(\mathbf{r}_i, \mathbf{r}_j), \quad (3.3)$$

$$\hat{V}(\mathfrak{R}) := \frac{1}{2} \sum_{\{l\mu\}, \{k\varrho\}} e_{l\mu} e_{k\varrho} C(\mathfrak{R}_{l\mu}, \mathfrak{R}_{k\varrho}). \quad (3.4)$$

The definitions for (3.2)–(3.4) are given in Section 1.

The perturbation  $\hat{K}^s$  is equal to the nondiagonal part of the adiabatic energy operator  $\hat{h}(\mathfrak{R}, \mathbf{r})$  and arises by the minimalization of  $\hat{h}(\mathfrak{R}, \mathbf{r})$  with the antisymmetric wave function of all electrons in state  $n$

$$|\chi_n\rangle = \left( \frac{1}{(N+s)!} \right)^{1/2} \sum_{\lambda_1 \dots \lambda_{N+s}} (-1)^p \cdot [\psi_{\eta_1}(\mathbf{r}_{\lambda_1}) \dots \psi_{\eta_s}(\mathbf{r}_{\lambda_s}) a_{\alpha_{k+1}^1}^n(\mathbf{r}_{\lambda_{s+1}}) \dots a_{\alpha_{k+M}^n}^n(\mathbf{r}_{\lambda_{N+s}})], \quad (3.5)$$

where the one electronic functions are defined in Section 1. These one particle functions are assumed to be orthogonal to each other with respect to the same electronic state  $n$ .

Ionic crystals have a relatively large energy gap between valence and conduction band of several ( $> 5$ ) eV. Therefore, we restrict ourselves to processes between impurities and the conduction band by assuming:

a) There are no direct excitation of regular shell electrons:

$$a_{\alpha_{l\mu}}^n \equiv a_{\alpha'_{l\mu}}^n.$$

b) All shells of the lattice ions are closed.

For various states of the impurity center electrons small modifications of the electronic shell functions respectively of their electronic moments are induced. They are important for state calculations. But for transitions we neglect these slight modifications and assume:

c) In a first approximation these shell functions remain unaltered:

$$a_{\alpha_{l\mu}}^n \equiv a_{\alpha'_{l\mu}}^n.$$

Then we have the following assumptions:

$$\begin{aligned} \langle a_{\alpha_{l\mu}}^n | a_{\beta_{k\varrho}}^{n'} \rangle &= \delta_{l\mu, k\varrho} \delta_{\alpha, \beta} \delta_{nn'}, \\ \langle \psi_{\eta} | a_{\alpha_{l\mu}}^{n'} \rangle &= 0 \quad \text{for all } l\mu, k\varrho, \alpha, \beta, n, n', \\ \langle \psi_{\eta'} | a_{\alpha_{l\mu}}^n \rangle &= 0. \end{aligned} \quad (3.6)$$

With these relations we extend the orthogonality of the one particle functions for a single electronic Hartree-Fock state to different Hartree-Fock states  $n$  and  $n'$ .

If we take into account the definitions (1.1), (1.2), (1.7), (1.21) and the assumptions (3.6) we get after some calculations for the perturbation operator (2.13):

$$\begin{aligned} \hat{K}^s(\mathfrak{R}) &= \sum_{i=1}^s \prod_{\substack{\alpha=1 \\ \alpha \neq i}}^s \delta_{\eta_{\alpha} \eta'_{\alpha}} \left\{ \left\langle \psi_{\eta_i}(\mathbf{r}) \right| -\frac{\hbar^2}{2m} \Delta_{\eta} \left| \psi_{\eta'_i}(\mathbf{r}) \right\rangle \right. \\ &\quad + \sum_{\{l\mu\}} e \langle \psi_{\eta_i}(\mathbf{r}) | [(m_{l\mu}^n \cdot \nabla_{l\mu}) \\ &\quad + a_{l\mu}(1 + \mathfrak{M}_{l\mu}^n \cdot \nabla_{l\mu})] C(\mathbf{r}, l\mu) | \psi_{\eta'_i}(\mathbf{r}) \rangle \\ &\quad + \sum_{\{l\mu\} \alpha_{l\mu}} \langle \psi_{\eta_i}(\mathbf{r}) a_{\alpha_{l\mu}}^n(\mathbf{r}') | e^2 C(\mathbf{r}, \mathbf{r}') \\ &\quad \cdot | \psi_{\eta'_i}(\mathbf{r}') a_{\alpha_{l\mu}}^n(\mathbf{r}') \rangle \Big\} \\ &\quad + \frac{1}{2} \sum_{i,j=1}^s \prod_{\substack{\alpha=1 \\ \alpha \neq i, j}}^s \delta_{\eta_{\alpha} \eta'_{\alpha}} [\langle \psi_{\eta_i}(\mathbf{r}) \psi_{\eta_j}(\mathbf{r}') | e^2 C(\mathbf{r}, \mathbf{r}') | \\ &\quad \cdot \{ \psi_{\eta'_i}(\mathbf{r}) \psi_{\eta'_j}(\mathbf{r}') - \psi_{\eta'_i}(\mathbf{r}') \psi_{\eta'_j}(\mathbf{r}) \} \rangle]. \end{aligned} \quad (3.7)$$

In (3.7) the multipole expansion of the Coulomb potential has been used.

This operator causes one and two particle transitions respectively. So we have to distinguish between the following two cases:

a) For one particle transitions there must hold the following conditions for the electronic quantum numbers  $\eta \in \mathbb{M}$  (1.18):

$$\eta_l \neq \eta_{l'} \quad \text{for one } l \in \{1, \dots, s\}. \quad (3.8)$$

For these transitions we can define the following operators:

$$\hat{k}_{\text{kin}}^s := \langle \psi_\eta(\mathbf{r}) | -\frac{\hbar^2}{2m} \Delta | \psi_{\eta'}(\mathbf{r}) \rangle, \quad (3.9)$$

$$\hat{k}_{\text{Phon}}^s := \sum_{\langle l\mu \rangle} e a_{l\mu} \langle \psi_\eta | (1 + \mathfrak{M}_{l\mu}^n \cdot \nabla_{l\mu}) C(\mathbf{r}, l\mu) | \psi_{\eta'} \rangle, \quad (3.10)$$

$$\hat{k}_{\text{Dip}}^s := \sum_{\langle l\mu \rangle} e \langle \psi_\eta | m_{l\mu} \cdot \nabla_{l\mu} C(\mathbf{r}, l\mu) | \psi_{\eta'} \rangle, \quad (3.11)$$

$$\hat{k}_{\text{ex}}^s := \sum_{\langle l\mu \rangle a_{l\mu}} e^2 \langle \psi_\eta(\mathbf{r}) a_{a_{l\mu}}^n(\mathbf{r}') | C(\mathbf{r}, \mathbf{r}') | a_{a_{l\mu}}^n(\mathbf{r}) \psi_{\eta'}(\mathbf{r}') \rangle. \quad (3.12)$$

The meanings of these operators are obvious:

- $\hat{k}_{\text{kin}}^s$  represents a kinetic operator for the impurity electrons;
- $\hat{k}_{\text{phon}}^s$  is the electron phonon interaction operator;
- $\hat{k}_{\text{dip}}^s$  contains the interactions of the electronic dipoles of the ions with the impurity states, and
- $\hat{k}_{\text{ex}}^s$  represents the exchange potential of the core electrons with the impurities.

b) For two particle transitions we have:

There are two inequalities of the electronic quantum numbers

$$\eta_l \neq \eta_{l'} \quad \text{and} \quad \eta_k \neq \eta_{k'} \quad \text{for } l, k \in \{1, \dots, s\}, \quad l \neq k. \quad (3.13)$$

Thereby (3.7) goes over into:

$$\hat{k}_A^s(\mathfrak{R}) := \langle \psi_\eta(\mathbf{r}) \psi_\varkappa(\mathbf{r}') | e^2 C(\mathbf{r}, \mathbf{r}') | \psi_{\eta'}(\mathbf{r}) \psi_{\varkappa'}(\mathbf{r}') \rangle - \langle \psi_\eta(\mathbf{r}) \psi_\varkappa(\mathbf{r}') | e^2 C(\mathbf{r}, \mathbf{r}') | \psi_{\eta'}(\mathbf{r}') \psi_{\varkappa'}(\mathbf{r}) \rangle \quad (3.14)$$

with  $\eta, \varkappa \in \mathbb{M}$ .

Our aim is to evaluate the Auger operator for the complete adiabatic crystal states  $nm$  defined in (2.3). The total Auger transition probabilities are given with (2.12), (2.22) and (3.14) by:

$$W_{nn'}^A = \frac{2\pi}{\hbar} Z_{\text{Phon}}^{-1} \sum_{m, m'} \exp\{-\beta E_{m'}^{n'}\} \cdot |\langle n m | \hat{k}_A^s | n' m' \rangle|^2 \delta(E_m^n - E_{m'}^{n'}). \quad (3.15)$$

The above operator (3.14) is well known in literature. However, we have given here a new deductive derivation for it in order to see which electronic

functions must be used. These functions have been calculated by Schmid [20] and Renn [6] explicitly.

In many papers the following screened Coulomb potential has been used for the Auger transitions:

$$C^{sc}(\mathbf{r}, \mathbf{r}') := \frac{\exp\{-\delta |\mathbf{r} - \mathbf{r}'|\}}{\varepsilon |\mathbf{r} - \mathbf{r}'|}. \quad (3.16)$$

But clearly we must use the pure Coulomb potential for our calculations, because in our theory the screening has been taken into account in the electronic and ionic multipole expressions explicitly [6].

#### 4. Phonon Assisted Auger Transitions

To derive phonon assisted transition probabilities, we have to use the dynamical electronic wave functions which can be written [7, 21]

$$\begin{aligned} \psi_\eta(\mathbf{r}, \mathfrak{R}) &= \psi_\eta(\mathbf{r}, \alpha^\eta(X^n)) \\ &= \sum_{\nu=0}^{\infty} \frac{1}{\nu!} \sum_{\{l^{\nu\mu^1}\}} \cdots \sum_{\{l^{\nu\mu^\nu}\}} X_{l^{\nu\mu^1}}^n \cdots X_{l^{\nu\mu^\nu}}^n \\ &\quad \cdot \left\{ \frac{\partial}{\partial X_{l^{\nu\mu^1}}^n} \cdots \frac{\partial}{\partial X_{l^{\nu\mu^\nu}}^n} \psi_\eta(\mathbf{r}, \alpha^\eta(X^n)) \right\}_{X^n=0} \end{aligned} \quad (4.1)$$

with the definition (1.3) and  $\alpha^\eta$  as variational parameter for the minimalisation. Concerning their derivation we refer to Stumpf [1, 21].

If we transform the displacements  $X_{l\mu}^n$  to the normal coordinates  $q_t^n$  (1.22), (4.1) goes over into [7]:

$$\psi_\eta(\mathbf{r}, q^n) = \sum_{\nu=0}^{\infty} \frac{1}{\nu!} \sum_{\{t_1\} \dots \{t_\nu\}} q_{t_1}^n \cdots q_{t_\nu}^n f_{t_1 \dots t_\nu}^\eta(\mathbf{r}). \quad (4.2)$$

In the following we use (4.2) for our representation of the electronic state and the relations

$$q_t^{n'} = q_t^n + a_t^{nn'} \quad \text{for all } t \quad (4.3)$$

for the normal coordinate displacements between different electronic states.

The relations (4.3) can formally be written down for ionic crystals [21]. For other semiconductor crystals these relations have to be proved.

For ionic crystals these displacements are restricted to a small number [21]. For the computation this restriction is very convenient, since with increasing number of normal coordinate displacements the numeric calculations increase also considerably.

This fact can be justified physically by the localization [20] of the impurity mode. Consequent-

ly, we restrict (4.3) to:

$$q_t^{\eta'} = q_t^{\eta} + a_t^{\eta\eta'}, \quad 1 \leq t \leq d_{\eta}; \quad q_t^{\eta'} = q_t^{\eta} \quad \text{for all other } t, \quad \eta \in \mathbb{M}. \quad (4.4)$$

Let us now define the following electronic matrix elements:

$$eA_{s'_1 \dots s'_{\mu'}, s_1 \dots s_{\mu}}^{t_1 \dots t_{\nu}} := \frac{1}{\nu! \mu! \nu'! \mu'!} \langle f_{t_1 \dots t_{\nu}}^{\eta}(\mathbf{r}) f_{s_1 \dots s_{\mu}}^{\kappa}(\mathbf{r}') | e^2 C(\mathbf{r}, \mathbf{r}') | f_{t'_1 \dots t'_{\nu'}}^{\mu'}(\mathbf{r}) f_{s'_1 \dots s'_{\mu'}}^{\kappa'}(\mathbf{r}') \rangle, \quad (4.5)$$

$$\text{ex}A_{s'_1 \dots s'_{\mu'}, s_1 \dots s_{\mu}}^{t_1 \dots t_{\nu}} := \frac{1}{\nu! \mu! \nu'! \mu'!} \langle f_{t_1 \dots t_{\nu}}^{\eta}(\mathbf{r}) f_{s_1 \dots s_{\mu}}^{\kappa}(\mathbf{r}') | e^2 C(\mathbf{r}, \mathbf{r}') | f_{t'_1 \dots t'_{\nu'}}^{\eta'}(\mathbf{r}') f_{s'_1 \dots s'_{\mu'}}^{\kappa'}(\mathbf{r}') \rangle \quad (4.6)$$

which hold for the Coulomb and exchange interaction. For the Auger matrix element (2.12) with the definition (1.28) and the dynamical electron wave function (4.2) we get:

$$K_{\eta\kappa, \eta'\kappa'}^s = \Delta_{\eta\kappa, \eta'\kappa'} \sum_{m, m'} \sum_{\substack{\nu, t_1 \dots t_{\nu} \\ \nu', t'_1 \dots t'_{\nu'}}} \sum_{\substack{\mu, s_1 \dots s_{\mu} \\ \mu', s'_1 \dots s'_{\mu'}}} \left[ eA_{s'_1 \dots s'_{\mu'}, s_1 \dots s_{\mu}}^{t_1 \dots t_{\nu}} - \text{ex}A_{s'_1 \dots s'_{\mu'}, s_1 \dots s_{\mu}}^{t_1 \dots t_{\nu}} \right] \cdot \langle \varphi_m^n | (q_{t_1}^{\eta} \dots q_{t_{\nu}}^{\eta}) (q_{s_1}^{\kappa} \dots q_{s_{\mu}}^{\kappa}) (q_{t'_1}^{\eta'} \dots q_{t'_{\nu'}}^{\eta'}) (q_{s'_1}^{\kappa'} \dots q_{s'_{\mu'}}^{\kappa'}) | \varphi_{m'}^{n'} \rangle. \quad (4.7)$$

The normal coordinate polynomials can be expressed by generating functions. We introduce the operator

$$\hat{A} := \Delta_{\eta\kappa, \eta'\kappa'} \sum_{m, m'} \sum_{\substack{\nu, t_1 \dots t_{\nu} \\ \nu', t'_1 \dots t'_{\nu'}}} \sum_{\substack{\mu, s_1 \dots s_{\mu} \\ \mu', s'_1 \dots s'_{\mu'}}} \left[ eA_{s'_1 \dots s'_{\mu'}, s_1 \dots s_{\mu}}^{t_1 \dots t_{\nu}} - \text{ex}A_{s'_1 \dots s'_{\mu'}, s_1 \dots s_{\mu}}^{t_1 \dots t_{\nu}} \right] \prod_{i=1}^{\nu} \frac{\partial}{\partial \varrho_{t_i}} \prod_{i=1}^{\mu} \frac{\partial}{\partial \bar{\varrho}_{s_i}} \prod_{i=1}^{\nu'} \frac{\partial}{\partial \varrho'_{t'_i}} \prod_{i=1}^{\mu'} \frac{\partial}{\partial \bar{\varrho}'_{s'_i}} \quad (4.8)$$

and the expression (4.7) then reads

$$K_{\eta\kappa, \eta'\kappa'}^s = \hat{A} \left\langle \varphi_m^n \left| \exp \left\{ \sum_{\{t\}} q_t^{\eta} \varrho_t + \sum_{\{s\}} q_s^{\kappa} \bar{\varrho}_s + \sum_{\{t'\}} q_{t'}^{\eta'} \varrho'_{t'} + \sum_{\{s'\}} q_{s'}^{\kappa'} \bar{\varrho}'_{s'} \right\} \right| \varphi_{m'}^{n'} \right\rangle. \quad (4.9)$$

Observing (4.3), (4.4) resp., and introducing the following new parameters

$$\gamma_t := \varrho_t + \varrho'_t \quad \text{and} \quad \bar{\gamma}_s := \bar{\varrho}_s + \bar{\varrho}'_s \quad (4.10)$$

we obtain from (4.9):

$$K_{\eta\kappa, \eta'\kappa'}^s = \hat{A} \exp \left\{ \sum_{\{t\}} a_t^{\eta\eta'} (\gamma_t - \varrho_t) + \sum_{\{s\}} a_s^{\kappa\kappa'} (\bar{\gamma}_s - \bar{\varrho}_s) \right\} \langle \varphi_m^n | \exp \left\{ \sum_{\{t\}} q_t^{\eta'} \gamma_t + \sum_{\{s\}} q_s^{\kappa'} \bar{\gamma}_s \right\} | \varphi_{m'}^{n'} \rangle. \quad (4.11)$$

The Auger transition probabilities in the Pauli Master equation (2.22) then have the following form:

$$W_{nn'}^A(T) = \hat{A} \hat{A}^* \exp \left\{ \sum_{\{t\}} [(\gamma_t - \varrho_t) + (\gamma_t^* - \varrho_t^*)] a_t^{\eta\eta'} + \sum_{\{s\}} [(\bar{\gamma}_s - \bar{\varrho}_s) + (\bar{\gamma}_s^* - \bar{\varrho}_s^*)] a_s^{\kappa\kappa'} \right\} \mathbf{\Gamma}(T) |_0. \quad (4.12)$$

In this expression, the phonon part of the transitions is collected in

$$\mathbf{\Gamma}(T) := \frac{2\pi}{\hbar} Z_{\text{Phon}}^{-1} \sum_{m, m'} \exp \{ -\beta E_{m'}^{\eta'} \} \langle \varphi_m^n | \exp \left\{ \sum_{\{t\}} q_t^{\eta'} \gamma_t + \sum_{\{s\}} q_s^{\kappa'} \bar{\gamma}_s \right\} | \varphi_{m'}^{n'} \rangle \cdot \langle \varphi_{m'}^{n'} | \exp \left\{ \sum_{\{t\}} q_t^{\eta'} \gamma_t^* + \sum_{\{s\}} q_s^{\kappa'} \bar{\gamma}_s^* \right\} | \varphi_m^n \rangle \delta(E_m^n - E_{m'}^{\eta'}) \quad (4.13)$$

where the  $\gamma_t^*$ ,  $\bar{\gamma}_t^*$  respectively are not the complex conjugates of  $\gamma_t$  and  $\bar{\gamma}_t$  respectively, but are new parameters. The operator  $\hat{A}$  does not represent the adjoint operator of  $\hat{A}$  therefore. Rather the star means that there are used the new parameters  $\gamma_t^*$ ,  $\bar{\gamma}_t^*$ .

These transition probabilities have resonance character [4] which is due to the dressed phonons [2]. The eigenstate equation of the dressed phonons is:

$$\hat{D}_{n'} | \varphi_{m'}^{n'} \rangle = E_{m'}^{\eta'} | \varphi_{m'}^{n'} \rangle. \quad (4.14)$$

If we restrict ourselves to the diagonal approximation for the initial harmonic phonons  $|\Phi_m^{n'}\rangle$  and final harmonic phonons  $|\Phi_m^n\rangle$ , then the phonon part of (4.12) becomes [7]:

$$\begin{aligned} \Gamma(T) = & \frac{1}{\hbar} Z_{\text{Phon}}^{-1} \sum_{m, m'} \exp \{-\beta \bar{E}_m^n\} \langle \Phi_m^n | \exp \left\{ \sum_{\{t\}} q_t^{n'} \gamma_t + \sum_{\{s\}} q_s^{n'} \bar{\gamma}_s \right\} | \Phi_m^{n'} \rangle \\ & \cdot \langle \Phi_m^{n'} | \exp \left\{ \sum_{\{t\}} q_t^{n'} \gamma_t^* + \sum_{\{s\}} q_s^{n'} \bar{\gamma}_s^* \right\} | \Phi_m^n \rangle \frac{\gamma_m^{n'}}{(\bar{E}_m^n - \bar{E}_m^{n'} - \Delta_m^{n'})^2 + \frac{1}{4} (\gamma_m^{n'})^2} . \end{aligned} \quad (4.15)$$

In this formula the Lorentz factor will be approximated by the soft  $\delta_\gamma$  if we neglect the energy displacements  $\Delta_m^{n'}$  and take for the individual half width  $\gamma_m^{n'}$  a thermally averaged width  $\gamma(T)$  [22]:

$$\delta_\gamma(\bar{E}_m^n - \bar{E}_m^{n'}) := \frac{1}{2\pi} \frac{\gamma(T)}{(\bar{E}_m^n - \bar{E}_m^{n'})^2 + \frac{1}{4} \gamma^2(T)} . \quad (4.16)$$

We further assume that the  $d_\eta$  normal coordinates coupled to the impurity electron  $\eta$  are different from those of the impurity center  $\kappa$ :

$$\{q_1^\kappa \dots q_{d_\kappa}^\kappa\} \neq \{q_1^\eta \dots q_{d_\eta}^\eta\} . \quad (4.17)$$

This can be justified physically by the impurity concentrations in the crystal if the impurities are so far of each other that there is no overlapping of the localized modes coupled to the impurities. So we get:

$$\begin{aligned} \Gamma(T) = & \frac{2\pi}{\hbar} Z_{\text{phon}}^{-1} \sum_{mm'} \exp \{-\beta \bar{E}_m^n\} \delta_\gamma(\bar{E}_m^n - \bar{E}_m^{n'}) \prod_{t=1}^{d_\eta} \langle \Phi_{m_t^\eta}^\eta | \exp \{q_t^{n'} \gamma_t\} | \Phi_{m_t^\eta}^{n'} \rangle \\ & \cdot \langle \Phi_{m_t^\eta}^{n'} | \exp \{q_t^{n'} \gamma_t^*\} | \Phi_{m_t^\eta}^\eta \rangle \prod_{s=1}^{d_\kappa} \langle \Phi_{m_s^\kappa}^\kappa | \exp \{q_s^{n'} \bar{\gamma}_s\} | \Phi_{m_s^\kappa}^{n'} \rangle \langle \Phi_{m_s^\kappa}^{n'} | \exp \{q_s^{n'} \bar{\gamma}_s^*\} | \Phi_{m_s^\kappa}^\kappa \rangle . \end{aligned} \quad (4.18)$$

If we use the Fourier transformation of the Lorentz function and observe the decompositions of the total lattice energy (1.27)

$$\bar{E}_m^n = e_m^n + U_n^{\text{st}}, \quad \bar{E}_m^{n'} = e_m^{n'} + U_n^{\text{st}} \quad (4.19)$$

with

$$e_m^n = \sum_{i=1}^{d_\eta} (m_i^\eta + \frac{1}{2}) \hbar \omega_i^\eta + \sum_{i=1}^{d_\kappa} (m_i^\kappa + \frac{1}{2}) \hbar \omega_i^\kappa + \tilde{e}_m^n , \quad (4.20)$$

$$e_m^{n'} = \sum_{i=1}^{d_\eta} (m_i^{n'} + \frac{1}{2}) \hbar \omega_i^{n'} + \sum_{i=1}^{d_\kappa} (m_i^{n'} + \frac{1}{2}) \hbar \omega_i^{n'} + \tilde{e}_m^{n'} \quad (4.21)$$

then the expression (4.18) goes over into

$$\Gamma(T) = \frac{2\pi}{\hbar} \int \exp \{i \tau \Delta U_{nn'}^{\text{st}}\} \cdot \exp \{-i \gamma | \tau | \} \tilde{\Gamma}^{\eta\eta'}(T) \tilde{\Gamma}^{\kappa\kappa'}(T) d\tau \quad (4.22)$$

with the definitions:

$$\Delta U_{nn'}^{\text{st}} := U_n^{\text{st}} - U_{n'}^{\text{st}}, \quad (\text{static electronic energy difference}), \quad (4.23)$$

$$\begin{aligned} \tilde{\Gamma}^{\eta\eta'}(T) := & \prod_{t=1}^{d_\eta} \exp \left\{ \frac{i \tau}{2} \hbar (\omega_t^\eta - \omega_t^{n'}) \right\} [1 - \exp \{-\beta \hbar \omega_t^{n'}\}] \sum_{m_t^\eta, m_t^{n'}} \exp \{-\beta m_t^\eta \hbar \omega_t^\eta + i \hbar \tau (m_t^\eta \omega_t^\eta \\ & - m_t^{n'} \omega_t^{n'})\} \langle \Phi_{m_t^\eta}^\eta | \exp \{q_t^{n'} \gamma_t\} | \Phi_{m_t^\eta}^{n'} \rangle \langle \Phi_{m_t^\eta}^{n'} | \exp \{q_t^{n'} \gamma_t^*\} | \Phi_{m_t^\eta}^\eta \rangle , \end{aligned} \quad (4.24)$$

$$\begin{aligned} \tilde{\Gamma}^{\kappa\kappa'}(T) := & \prod_{t=1}^{d_\kappa} \exp \left\{ \frac{i \tau}{2} \hbar (\omega_t^\kappa - \omega_t^{n'}) \right\} [1 - \exp \{-\beta \hbar \omega_t^{n'}\}] \sum_{m_t^\kappa, m_t^{n'}} \exp \{-\beta m_t^\kappa \hbar \omega_t^\kappa + i \hbar \tau (m_t^\kappa \omega_t^\kappa \\ & - m_t^{n'} \omega_t^{n'})\} \langle \Phi_{m_t^\kappa}^\kappa | \exp \{q_t^{n'} \bar{\gamma}_t\} | \Phi_{m_t^\kappa}^{n'} \rangle \langle \Phi_{m_t^\kappa}^{n'} | \exp \{q_t^{n'} \bar{\gamma}_t^*\} | \Phi_{m_t^\kappa}^\kappa \rangle \end{aligned} \quad (4.25)$$

and the equality of  $\tilde{e}_m^n$  and  $\tilde{e}_m^{n'}$ .

Analytically, the expressions (4.24) and (4.25) are identical, so we can restrict ourselves to one for the further evaluation.

We now apply the results of Koide [23] for the transformation dependency between different harmonic lattice states [see definitions (1.30)–(1.36)]:

$$|\Phi_{m_t^n}^{\eta'}\rangle = c_{m_t^n}^{-1} \hat{U}_t^\eta \hat{V}_t^\eta |\Phi_{m_t^n}^{\eta'}\rangle. \quad (4.26)$$

The equation for the occupation operator  $\hat{m}_t^{\eta'}$  has the form

$$\hat{m}_t^{\eta'} |\Phi_{m_t^n}^{\eta'}\rangle = m_t^{\eta'} |\Phi_{m_t^n}^{\eta'}\rangle \quad (4.27)$$

and their functional transformation behaviour of this operator is:

$$F(\hat{m}_t^{\eta'}) = \hat{U}_t^\eta \hat{V}_t^\eta F(\hat{m}_t^\eta) (\hat{U}_t^\eta)^{-1} (\hat{V}_t^\eta)^{-1}. \quad (4.28)$$

With (4.26), (4.27) and (4.28) we get for (4.24) and (4.25) resp. the result

$$\begin{aligned} \tilde{\mathbf{\Gamma}}^{\eta\eta'}(T) &= \prod_{t=1}^{d_\eta} \exp \left\{ \frac{i\tau}{2} \hbar (\omega_t^\eta - \omega_t^{\eta'}) \right\} [1 - \exp \{-\beta \hbar \omega_t^{\eta'}\}] \sum_{m_t^\eta} \exp \{-\beta m_t^\eta \hbar \omega_t^\eta + i\tau \hbar m_t^\eta \omega_t^\eta\} \\ &\cdot \langle \Phi_{m_t^n}^{\eta'} | \exp \{q_t^{\eta'} \gamma_t\} \hat{U}_t^\eta \hat{V}_t^\eta \exp \{-i\tau \hbar m_t^\eta \omega_t^\eta\} (\hat{U}_t^\eta)^{-1} (\hat{V}_t^\eta)^{-1} \exp \{q_t^{\eta'} \gamma_t^*\} | \Phi_{m_t^n}^{\eta'} \rangle. \end{aligned} \quad (4.29)$$

The first expression can be expressed as [7, 24]

$$\mathbf{\Gamma}^{\eta\eta'}(T) = \exp \left\{ \frac{i\tau}{2} \sum_{t=1}^{d_\eta} \hbar (\omega_t^\eta - \omega_t^{\eta'}) \right\} \prod_{t=1}^{d_\eta} \exp \{N_t^{\eta\eta'}\} \exp \{P_t^{\eta\eta'}\}. \quad (4.30)$$

We have used the following definitions [with subsidiary definitions (1.37)–(1.44)]:

$$\begin{aligned} \exp \{N_t^{\eta\eta'}\} &:= \exp \left\{ \frac{2 \exp \{-\beta \hbar \omega_t^{\eta'}\}}{1 - \exp \{-\beta \hbar \omega_t^{\eta'}\}} (d_{1,t}^{\eta\eta'} d_{2,t}^{\eta\eta'} + d_{1,t}^{\eta\eta'*} d_{2,t}^{\eta\eta'*}) + \frac{1}{2} (d_{3,t}^{\eta\eta'} + d_{3,t}^{\eta\eta'*}) \right\} \\ &\cdot \exp \left\{ \frac{\exp \{-\beta \hbar \omega_t^{\eta'}\}}{1 - \exp \{-\beta \hbar \omega_t^{\eta'}\}} (d_{1,t}^{\eta\eta'} d_{1,t}^{\eta\eta'*}) \exp \{i\tau \hbar \omega_t^\eta\} \right\} \\ &\cdot \exp \left\{ \frac{1}{1 - \exp \{-\beta \hbar \omega_t^{\eta'}\}} (d_{2,t}^{\eta\eta'} d_{2,t}^{\eta\eta'*}) \exp \{-i\tau \hbar \omega_t^\eta\} \right\} \end{aligned} \quad (4.31)$$

$$\exp \{P_t^{\eta\eta'}\} := \exp \{f_{0,t}^{\eta\eta'}\} \sum_{v_t} g_{v_t}^{\eta\eta'} \exp \{i\tau v_t \hbar \omega_t^{\eta'}\}. \quad (4.32)$$

The expressions (4.31) and (4.32) are not very appropriate for further calculations; so we introduce new definitions:

$$\begin{aligned} \sigma_t^{\eta\eta'}(\mu_t, T) &:= \exp \left\{ \frac{\exp \{-\beta \hbar \omega_t^{\eta'}\}}{1 - \exp \{-\beta \hbar \omega_t^{\eta'}\}} (d_{1,t}^{\eta\eta'} d_{2,t}^{\eta\eta'} + d_{1,t}^{\eta\eta'*} d_{2,t}^{\eta\eta'*}) + \frac{1}{2} (d_{3,t}^{\eta\eta'} + d_{3,t}^{\eta\eta'*}) \right\} \\ &\cdot \sum_{\varrho} \frac{(c_t^{\eta\eta'})^{e+\mu_t} (b_t^{\eta\eta'})^e}{(\varrho + \mu_t)! \varrho!}, \end{aligned} \quad (4.33)$$

$$\Delta E_{\eta\eta'} := \Delta U_{\eta\eta'}^{st} + \frac{1}{2} \sum_{t=1}^{d_\eta} \hbar (\omega_t^\eta - \omega_t^{\eta'}). \quad (4.34)$$

Remembering that  $\Delta U_{nn'}^{st}$  can be expressed as

$$\Delta U_{nn'}^{st} = \Delta U_{\eta\eta'}^{st} + \Delta U_{\kappa\kappa'}^{st} \quad (4.35)$$

we can integrate the expression (4.21) and get the final result for the phonon part of the Auger transitions:

$$\begin{aligned} \mathbf{\Gamma}(T) &= \frac{2\pi}{\hbar} \left( \exp \left\{ \sum_{t=1}^{d_\eta} f_{0,t}^{\eta\eta'} \right\} \sum_{\mu_1 \dots \mu_{d_\eta}} \prod_{t=1}^{d_\eta} \sigma_t^{\eta\eta'}(\mu_t, T) \sum_{v_1 \dots v_{d_\eta}} g_{v_1}^{\eta\eta'} \dots g_{v_{d_\eta}}^{\eta\eta'} \right) \left( \exp \left\{ \sum_{t=1}^{d_\kappa} f_{0,t}^{\kappa\kappa'} \right\} \sum_{\bar{\mu}_1 \dots \bar{\mu}_{d_\kappa}} \prod_{t=1}^{d_\kappa} \sigma_t^{\kappa\kappa'}(\bar{\mu}_t, T) \right. \\ &\cdot \sum_{\bar{v}_1 \dots \bar{v}_{d_\kappa}} g_{\bar{v}_1}^{\kappa\kappa'} \dots g_{\bar{v}_{d_\kappa}}^{\kappa\kappa'} \Big) \cdot \delta_\gamma \left( \left[ \Delta E_{\eta\eta'} - \sum_{t=1}^{d_\eta} \hbar (\mu_t - v_t) \omega_t^{\eta'} \right] + \left[ \Delta E_{\kappa\kappa'} - \sum_{t=1}^{d_\kappa} \hbar (\bar{\mu}_t - \bar{v}_t) \omega_t^{\kappa'} \right] \right). \end{aligned} \quad (4.36)$$



With (3.36) and (4.12) we derived a calculable expression for phonon assisted Auger transitions. Now, if we know the special parameters occurring in our expression (4.36), e.g. the frequencies, the normal coordinate displacements, the physical factors, the electronic energy differences and the special electronic wave functions, we have the possibility to apply our result to different semiconductor models and substances.

For a final simplification of the above result we apply it to the special case of halogenid crystals with colour centers. Thereby, we assume in accordance with (4.3) in a first approximation that by the transition there will be no frequency shift of the coupled modes. The coupling of the impurities and the lattice can be expressed by one effective lattice mode and the whole expression (4.36) is reduced to

$$\mathbf{\Gamma}(T) = \frac{2\pi}{\hbar} \sum_{\mu} \sum_{\bar{\mu}} \sigma^{\eta\eta'}(\mu, T) \sigma^{\kappa\kappa'}(\bar{\mu}, T) \cdot \delta_{\gamma}(\Delta U_{nn'}^{st} - (\mu + \bar{\mu}) \hbar \omega^0). \quad (4.37)$$

The total Auger transition probabilities then read:

$$W_{nn'}^A(T) = \frac{2\pi}{\hbar} \hat{A} \hat{A}^* [\exp \{a^{\eta\eta'}[(\gamma - \varrho') + (\gamma^* - \varrho'^*)] + a^{\kappa\kappa'}[(\bar{\gamma} - \bar{\varrho}') + (\bar{\gamma}^* - \bar{\varrho}'^*)] \cdot \sum_{\mu} \sum_{\bar{\mu}} \sigma^{\eta\eta'}(\mu, T) \sigma^{\kappa\kappa'}(\bar{\mu}, T) \delta_{\gamma}(\Delta U_{nn'}^{st} - (\mu + \bar{\mu}) \hbar \omega^0)] | 0. \quad (4.38)$$

$$+ (\gamma^* - \varrho'^*)] + a^{\kappa\kappa'}[(\bar{\gamma} - \bar{\varrho}') + (\bar{\gamma}^* - \bar{\varrho}'^*)] \cdot \sum_{\mu} \sum_{\bar{\mu}} \sigma^{\eta\eta'}(\mu, T) \sigma^{\kappa\kappa'}(\bar{\mu}, T) \delta_{\gamma}(\Delta U_{nn'}^{st} - (\mu + \bar{\mu}) \hbar \omega^0)] | 0.$$

In a further approximation we restrict ourselves to the static coupling, since the Auger transitions are due to pure Coulomb interactions. Consequently the transition probability (4.38) is:

$$W_{nn'}^A(T) = \frac{2\pi}{\hbar} |\langle \psi_{\eta}(\mathbf{r}) \psi_{\kappa}(\mathbf{r}') | e^2 C(\mathbf{r}, \mathbf{r}') \cdot \langle \psi_{\eta'}(\mathbf{r}) \psi_{\kappa'}(\mathbf{r}') \rangle - \langle \psi_{\eta}(\mathbf{r}) \psi_{\kappa}(\mathbf{r}') | e^2 C(\mathbf{r}, \mathbf{r}') | \cdot \langle \psi_{\eta'}(\mathbf{r}') \psi_{\kappa'}(\mathbf{r}') \rangle |^2 \sum_{\mu} \sum_{\bar{\mu}} {}^0\sigma^{\eta\eta'}(\mu, T) {}^0\sigma^{\kappa\kappa'}(\bar{\mu}, T) \cdot \delta_{\gamma}(\Delta U_{nn'}^{st} - (\mu + \bar{\mu}) \hbar \omega^0) \quad (4.39)$$

${}^0\sigma^{\eta\eta'}$ ,  ${}^0\sigma^{\kappa\kappa'}$  results from  $\sigma^{\eta\eta'}$ ,  $\sigma^{\kappa\kappa'}$  by setting the parameters  $\gamma$ ,  $\gamma^*$  equal zero.

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