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THE GENERALIZED TRANSPORT EQUATION FOR AN ELECTRON

A SOLUTION IN A SIMPLE CASE

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Synopsis

The master equation to general order in the coupling responsible for the dissipative behaviour, derived in earlier papers by one of us (L.V.H.), is applied to the simple case of an electron in a system of randomly distributed, static, elastic scatterers. Replacing $W_{\boldsymbol{k}'}(\boldsymbol{k}, \boldsymbol{k}')$ by a constant, the equation can be solved approximately for general strength of the coupling. The solution, describing the approach to equilibrium of the electron momentum distribution, has an oscillatory character. The slightly more complicated case of an electron interacting with a vibrating harmonic lattice is also considered. It is shown how one can derive from the generalized master equation an equation describing the evolution of the electron alone, the phonons only entering through their coarse grained distribution in wave vector. Neglecting the phonon energies, one finds an equation of the same form as in the case of static, elastic scatterers.

1. *Introduction.* In three previous papers [1]) by one of us (L.V.H.), to be referred to as S, S′ and S″, the approach to equilibrium of a quantum many-body system has been studied. In these articles it was proved on the basis of a separation $H' = H + \lambda V$ of the Hamiltonian in unperturbed and perturbed terms and using certain properties of the perturbation, that the system tends to microcanonical equilibrium whenever its wave function at an initial time has random phases in the unperturbed representation. In S the theory was worked out under the supposition that the perturbation is weak. By so doing the well known master (or Pauli) equation was obtained in a more rigorous and satisfactory way than in usual derivations. In S′ and S″ the problem was treated to general order in the perturbation and a generalized master equation showing a memory effect was obtained.

Whereas the lowest order master or Pauli equation, describing the approach to equilibrium in the weak coupling limit, has been solved for a number of concrete physical situations, this is not the case with the generalized master equation derived in S′. It is well known that the Pauli

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equation describes a monotonic approach to equilibrium: the solution is always a superposition of non oscillating, exponentially decaying terms. For finite coupling, however, the time evolution of the probability distribution of the system toward equilibrium is not even qualitatively known. We therefore made it our main purpose to get some information on this time evolution by considering a simple case for which the problem could be handled to general order in the interaction. This is done in section 3 of the present paper, our working example being an electron in a system of randomly distributed, static, elastic scatterers. Our main conclusions will be that in the case of finite coupling the probability distribution shows damped oscillations in its approach to equilibrium. Preceding this discussion, section 2 presents for later reference a brief sketch of the general formalism.

To illustrate further the contents of the general theory we treat in section 4 a slightly more complicated system: an electron in a vibrating harmonic lattice. Our aim is there only to carry out for general electron-phonon coupling a calculation which is very familiar for weak coupling: the transformation of the master equation, which refers to the complete electron-lattice system, into a Boltzmann equation dealing with the electron alone. If phonon energies are neglected this generalized Boltzmann equation is of the type discussed and approximately solved in section 3.

2. *The master equation to general order.* For further reference we here recall briefly the derivation of the master equation to general order. For the details the reader may consult S'. We suppose that the Hamiltonian H' of the system is a sum of two terms

$$H' = H + \lambda V. \tag{2.1}$$

The eigenstates of H are exactly known and will be symbolized by $|\alpha\rangle$, where α represents the set of quantum numbers characterizing the state. Some of the quantum numbers have to be continuous in the limit of an infinite system. In this limit we adopt as normalization

$$\langle\alpha|\alpha'\rangle = \delta(\alpha - \alpha'), \tag{2.2}$$

the right hand side denoting a product of delta functions and Kronecker symbols for the continuous and discrete quantum numbers respectively. In the $|\alpha\rangle$ representation the perturbation λV has special properties, explained in detail in S'. They consist in the occurence of diagonal singularities of the form $\delta(\alpha - \alpha')$ in matrix elements $\langle\alpha|VA_1V \ldots A_nV|\alpha'\rangle$, where the A_j are diagonal in the $|\alpha\rangle$ representation. The matrix element $\langle\alpha|V|\alpha'\rangle$ has no such singularity.

We consider now the wave function $|\varphi_0\rangle$ of the system at time $t = 0$:

$$|\varphi_0\rangle = \int |\alpha\rangle \, \mathrm{d}\alpha c(\alpha). \tag{2.3}$$

We suppose $|\varphi_0\rangle$ to be normalized,

$$\langle\varphi_0|\varphi_0\rangle = \int |c(\alpha)|^2 \, d\alpha = 1. \tag{2.4}$$

If we choose units such that $\hbar = 1$, the wave function at time t is given by

$$\varphi_t = U_t\varphi_0 \tag{2.5}$$

$$U_t = \exp[-i(H + \lambda V)t]. \tag{2.6}$$

Let us now consider an operator A, diagonal in the $|\alpha\rangle$ representation, so that

$$A|\alpha\rangle = |\alpha\rangle A(\alpha) \tag{2.7}$$

and assume that $A(\alpha)$ is a smooth function of the continuous quantum numbers of $|\alpha\rangle$. By considering

$$\langle\varphi_t|A|\varphi_t\rangle = \int A(\alpha)\, p_t(\alpha)\, d\alpha, \tag{2.8}$$

we can introduce the (coarse grained) probability density $p_t(\alpha)$ of the system at time t. Inserting (2.5) and (2.6) into (2.8) and separating the diagonal singularity of the matrix element $\langle\alpha|U_{-t}AU_t|\alpha'\rangle$ one finds an expression of the form

$$\langle\varphi_t|A|\varphi_t\rangle = \langle\varphi_0|U_{-t}AU_t|\varphi_0\rangle = \int A(\alpha'')\, d\alpha'' \int P(t|\alpha''\alpha)\, d\alpha\, |c(\alpha)|^2 + \\ + \int A(\alpha'')\, d\alpha'' \int I(t|\alpha''\alpha\alpha')\, d\alpha\, d\alpha'\, c^*(\alpha)\, c(\alpha'), \tag{2.9}$$

where $I(t|\alpha''\alpha\alpha')$ has no $\delta(\alpha - \alpha')$ singularity. Since $A(\alpha)$ and $c(\alpha)$ are arbitrary, this equation entirely defines $P(t|\alpha''\alpha)$ and $I(t|\alpha''\alpha\alpha')$ in terms of the Hamiltonian and the $|\alpha\rangle$ representation. Comparing (2.8) and (2.9) one gets

$$p_t(\alpha'') = \int P(t|\alpha''\alpha)\, d\alpha\, |c(\alpha)|^2 + \int I(t|\alpha''\alpha\alpha')\, d\alpha\, d\alpha'\, c^*(\alpha)\, c(\alpha'). \tag{2.10}$$

For an initial state $|\varphi_0\rangle$ with "random" phases the second term on the right is negligible and we obtain

$$p_t(\alpha') = \int P(t|\alpha'\alpha)\, d\alpha\, |c(\alpha)|^2. \tag{2.11}$$

The quantity $P(t|\alpha'\alpha)$ can be interpreted as the (coarse grained) transition probability from α to α' in the time interval t. In S it has been calculated in the weak coupling limit ($\lambda \to 0$, $\lambda^2 t$ finite) and shown to be the solution of the Pauli (= lowest order) master equation, with initial condition $P(0|\alpha''\alpha) = \delta(\alpha'' - \alpha)$.

In S' the quantity $P(t|\alpha'\alpha)$ has been studied to general order in the perturbation λV. It was there shown that it is the integral

$$P(t|\alpha'\alpha) = \int_{-\infty}^{\infty} P_E(t|\alpha'\alpha)\, dE \tag{2.12}$$

of an energy dependent "partial transition probability" $P_E(t|\alpha'\alpha)$ which

obeys a generalized master equation of non-markovian type:

$$\frac{dP_E(t|\alpha\alpha_0)}{dt} = \delta(\alpha - \alpha_0)\, f_E(t|\alpha) + 2\pi\lambda^2 \int_0^t dt' \int w_E(t - t'|\alpha\alpha') \cdot$$
$$\cdot d\alpha' P_E(t'|\alpha'\alpha_0) - 2\pi\lambda^2 \int_0^t dt' \int d\alpha'\, w_E(t - t'|\alpha'\alpha)\, P_E(t'|\alpha\alpha_0). \quad (2.13)$$

We briefly recall how this result is obtained, and how the functions P_E, f_E and w_E are defined. As is well known the evolution operator U_t can be expressed with the help of the resolvent operator $R_l = (H' - l)^{-1}$. Using this connection one finds

$$P(t|\alpha'\alpha) = -(2\pi)^{-2} \int_\gamma dl \int_{\gamma'} dl' \exp[i(l - l')\, t]\, X_{ll'}(\alpha'\alpha). \quad (2.14)$$

The contours γ, γ' encircle the real axis counterclockwise. The function $X_{ll'}(\alpha'\alpha)$ is defined by the identity

$$\{R_l A R_{l'}\}_d |\alpha\rangle = |\alpha\rangle \int A(\alpha')\, d\alpha' X_{ll'}(\alpha'\alpha) \quad (2.15)$$

where the suffix d indicates the diagonal part of the matrix element (see S'). A straight perturbation expansion of $X_{ll'}(\alpha'\alpha)$ in λV would be poorly convergent for special values of l, l'. It is therefore useful to rewrite this quantity as a series

$$X_{ll'}(\alpha\alpha_0) = D_l(\alpha)\, D_{l'}(\alpha)\, \delta(\alpha - \alpha_0) + \lambda^2 D_l(\alpha)\, D_{l'}(\alpha) \cdot$$
$$\cdot [W_{ll'}(\alpha\alpha_0) + \lambda^2 \int W_{ll'}(\alpha\alpha_1) D_l(\alpha_1) D_{l'}(\alpha_1) d\alpha_1 W_{ll'}(\alpha_1\alpha_0) + \ldots] D_l(\alpha_0) D_{l'}(\alpha_0), \quad (2.16)$$

involving the diagonal part $D_l(\alpha)$ of the resolvent R_l and a new function $W_{ll'}(\alpha'\alpha)$. This function has the character of a transition rate and is defined in terms of an irreducible diagonal part (see S') *)

$$\{(V - \lambda V D_l V + \ldots)\, A\, (V - \lambda V D_{l'} V + \ldots)\}_{id} |\alpha\rangle = |\alpha\rangle \int A(\alpha')\, d\alpha' W_{ll'}(\alpha'\alpha) \quad (2.17)$$

for arbitrary diagonal A. Also D_l is conveniently rewritten in terms of another function

$$D_l = (H - l - \lambda^2 G_l)^{-1}. \quad (2.18)$$

G_l obeys the equation

$$G_l = \{V D_l V - \lambda V D_l V D_l V + \ldots\}_{id}. \quad (2.19)$$

Because of the occurrence of irreducible diagonal parts the convergence of the series involved in (2.17) and (2.19) does not depend critically on the particular values of l and l'. By taking (2.19) for two values of l and subtracting one obtains an important identity between $G_l(\alpha)$ and $W_{ll'}(\alpha\alpha')$:

$$G_l(\alpha) - G_{l'}(\alpha) = -i \int d\alpha' \tilde{W}_{ll'}(\alpha'\alpha), \quad (2.20)$$

with

$$\tilde{W}_{ll'}(\alpha'\alpha) = i[D_l(\alpha') - D_{l'}(\alpha')]\, W_{ll'}(\alpha'\alpha). \quad (2.21)$$

*) The irreducible diagonal part (suffix *id*) is obtained when all intermediate states are taken to be different from each other and from the initial state.

Using (2.18), the identity (2.20) implies

$$(l - l')\, D_l(\alpha)\, D_{l'}(\alpha) = D_l(\alpha) - D_{l'}(\alpha) + i\lambda^2 \int \mathrm{d}\alpha'\ \tilde{W}_{ll'}(\alpha'\alpha)\, D_l(\alpha)\, D_{l'}(\alpha), \quad (2.22)$$

a relation which can be converted into an equation for $X_{ll'}(\alpha'\alpha)$:

$$(l - l')\, X_{ll'}(\alpha\alpha_0) = [D_l(\alpha) - D_{l'}(\alpha)]\, \delta(\alpha - \alpha_0) - \\ - i\lambda^2 \int \tilde{W}_{ll'}(\alpha\alpha')\, \mathrm{d}\alpha'\, X_{ll'}(\alpha'\alpha_0) + i\lambda^2 \int \mathrm{d}\alpha'\, \tilde{W}_{ll'}(\alpha'\alpha)\, X_{ll'}(\alpha\alpha_0). \quad (2.23)$$

We now define the partial transition probability at energy E by

$$P_E(t\,|\,\alpha\alpha_0) = (2\pi^2)^{-1}\, s(t) \int_\gamma \mathrm{d}l\, \exp(2ilt)\, X_{E+l,E-l}(\alpha\alpha_0), \quad (2.24)$$

E being real and $t \neq 0$. $s(t)$ stands for $t^{-1}\,|t|$. As proved in S', (2.23) implies that $P_E(t\,|\,\alpha\alpha_0)$ verifies the equations (2.12) and (2.13) given above if the following definitions are adopted:

$$w_E(t\,|\,\alpha'\alpha) = (2\pi^2)^{-1} \int_\gamma \mathrm{d}l\, \exp(2ilt)\, \tilde{W}_{E+l,E-l}(\alpha'\alpha), \quad (2.25)$$

$$f_E(t\,|\,\alpha) = (2\pi^2)^{-1} i s(t) \int_\gamma \mathrm{d}l\, \exp(2ilt)\, [D_{E+l}(\alpha) - D_{E-l}(\alpha)]. \quad (2.26)$$

The generalized master equation (2.13) must be supplemented by the initial condition

$$P_E(0\,|\,\alpha\alpha_0) = 0 \quad (2.27)$$

required by the definition (2.24).

3. *A solution in a simple case.* We apply the general theory to a simple situation: an electron in a system of randomly distributed, static, elastic scattering centers. It is easy to prove that the formal properties of the perturbation are valid in this case (see e.g. ref. 2, Appendix). All equations of the general theory apply to this situation if the quantum numbers α are taken to be the three components of the wave vector $\boldsymbol{k}$ of the electron (the electron spin is neglected). In this special case the master equation to general order has the form of a Boltzmann equation. We call it the generalized Boltzmann equation for an electron in a system of random elastic scattering centers.

The equation (2.16) for the basic function $X_{ll'}(\alpha\alpha_0)$ becomes

$$X_{ll'}(\boldsymbol{k}\boldsymbol{k}_0) = D_l(\boldsymbol{k})\, D_{l'}(\boldsymbol{k})\, \delta(\boldsymbol{k} - \boldsymbol{k}_0) + \lambda^2 D_l(\boldsymbol{k})\, D_{l'}(\boldsymbol{k}) \cdot \\ \cdot [W_{ll'}(\boldsymbol{k}\boldsymbol{k}_0) + \lambda^2 \int W_{ll'}(\boldsymbol{k}\boldsymbol{k}_1)\, D_l(\boldsymbol{k}_1)\, D_{l'}(\boldsymbol{k}_1)\, \mathrm{d}\boldsymbol{k}_1\, W_{ll'}(\boldsymbol{k}_1\boldsymbol{k}_0) + \ldots] \cdot \\ \cdot D_l(\boldsymbol{k}_0)\, D_{l'}(\boldsymbol{k}_0). \quad (3.1)$$

We now make for $W_{ll'}(\boldsymbol{k}, \boldsymbol{k}')$ a very simple ansatz

$$W_{ll'}(\boldsymbol{k}, \boldsymbol{k}') = \begin{cases} W \text{ for } k, k' \leqslant a \\ 0 \text{ otherwise,} \end{cases} \quad (3.2)$$

with a and W given positive constants (k denotes the length of $\boldsymbol{k}$, and

similarly for k'). This admittedly very crude approximation has the great advantage to allow an explicit calculation of X, and consequently of the time evolution of the electron, for arbitrary strength of the interaction, i.e. to all orders in λ^2. Indeed, the series in (3.1) can now be summed explicitly with the result

$$X_{ll'}(\boldsymbol{k}\boldsymbol{k}_0) = D_l(\boldsymbol{k})\, D_{l'}(\boldsymbol{k})\, \delta(\boldsymbol{k} - \boldsymbol{k}_0) + \\ + \lambda^2 W D_l(\boldsymbol{k})\, D_{l'}(\boldsymbol{k})\, D_l(\boldsymbol{k}_0)\, D_{l'}(\boldsymbol{k}_0)\, [1 - \lambda^2 W \int \mathrm{d}\boldsymbol{k}_1 D_l(\boldsymbol{k}_1)\, D_{l'}(\boldsymbol{k}_1)]^{-1}. \quad (3.3)$$

In this and *all* further equations of this section we restrict *all* wave vectors to the region $k \leqslant a$; this applies in particular to the integration in (3.3) *).

The form of the function $D_l(\boldsymbol{k})$ under our ansatz (3.2) can be studied by applying (2.18), (2.20) and (2.21). The first of these equations gives

$$D_l(\boldsymbol{k}) = [\varepsilon_{\boldsymbol{k}} - l - \lambda^2 G_l(\boldsymbol{k})]^{-1} \quad (3.4)$$

where $\varepsilon_{\boldsymbol{k}}$ is the energy of a free electron of wave vector $\boldsymbol{k}$. An implicit equation for $G_l(\boldsymbol{k})$ is then obtained from (2.20) and (2.21) which under our ansatz give

$$G_l(\boldsymbol{k}) - G_{l'}(\boldsymbol{k}) = W \int \mathrm{d}\boldsymbol{k}' \, [D_l(\boldsymbol{k}') - D_{l'}(\boldsymbol{k}')]. \quad (3.5)$$

For $l' \to \infty$ both $G_{l'}(\boldsymbol{k})$ and $D_{l'}(\boldsymbol{k})$ approach zero and this relation becomes

$$G_l(\boldsymbol{k}) = W \int D_l(\boldsymbol{k}')\, \mathrm{d}\boldsymbol{k}' = W \int [\varepsilon_{\boldsymbol{k}'} - l - \lambda^2 G_l(\boldsymbol{k}')]^{-1}\, \mathrm{d}\boldsymbol{k}'$$

where (3.4) has been used; clearly $G_l(\boldsymbol{k})$ is independent of $\boldsymbol{k}$ and we may put

$$G_l(\boldsymbol{k}) = g_l \; **). \quad (3.6)$$

g_l is a solution of

$$g_l = 4\pi W \int_0^a (\varepsilon_{\boldsymbol{k}'} - l - \lambda^2 g_l)^{-1} k'^2 \, \mathrm{d}k'. \quad (3.7)$$

With the above equations (3.3) simplifies greatly. Notice that

$$D_l(\boldsymbol{k}_1)\, D_{l'}(\boldsymbol{k}_1) = (l + \lambda^2 g_l - l' - \lambda^2 g_{l'})^{-1} [D_l(\boldsymbol{k}_1) - D_{l'}(\boldsymbol{k}_1)]. \quad (3.8)$$

The integral in (3.3) therefore reduces to the one in (3.5), and (3.3) becomes

$$X_{ll'}(\boldsymbol{k}\boldsymbol{k}_0) = D_l(\boldsymbol{k})\, D_{l'}(\boldsymbol{k})\, \delta(\boldsymbol{k} - \boldsymbol{k}_0) + \lambda^2 W D_l(\boldsymbol{k})\, D_{l'}(\boldsymbol{k})\, D_l(\boldsymbol{k}_0)\, D_{l'}(\boldsymbol{k}_0) \cdot \\ \cdot [1 - \lambda^2 (g_l - g_{l'})(l + \lambda^2 g_l - l' - \lambda^2 g_{l'})^{-1}]^{-1}. \quad (3.9)$$

A new application of (3.8) gives the very simple result

$$X_{ll'}(\boldsymbol{k}\boldsymbol{k}_0) = \\ = \frac{D_l(\boldsymbol{k}) - D_{l'}(\boldsymbol{k})}{l - l' + \lambda^2 (g_l - g_{l'})} \left[\delta(\boldsymbol{k} - \boldsymbol{k}_0) + \lambda^2 W [D_l(\boldsymbol{k}_0) - D_{l'}(\boldsymbol{k}_0)]\, (l - l')^{-1} \right]. \quad (3.10)$$

Applying the transformation (2.24) we obtain the partial transition pro-

*) $X_{ll'}(\boldsymbol{k}\boldsymbol{k}_0)$ vanishes for $k \leqslant a$, $k_0 > a$ and $k \geqslant a$, $k_0 < a$. For $k > a$, $k_0 > a$ it has the unperturbed value $(\varepsilon_{\boldsymbol{k}} - l)^{-1}$. $(\varepsilon_{\boldsymbol{k}} - l)^{-1}\, \delta(\boldsymbol{k} - \boldsymbol{k}_0)$, where $\varepsilon_{\boldsymbol{k}}$ is the free electron energy.

**) As mentioned above our equations hold for k, $k' \leqslant a$; $G_l(\boldsymbol{k})$ vanishes for $k > a$.

bability $P_E(t|\boldsymbol{k}\boldsymbol{k}_0)$ to general order. For $t > 0$ this formula becomes

$$P_E(t|\boldsymbol{k}\boldsymbol{k}_0) = (2\pi^2)^{-1}\int_\gamma \mathrm{d}l \exp(2ilt)\,\frac{D_{E+l}(\boldsymbol{k}) - D_{E-l}(\boldsymbol{k})}{2l + \lambda^2[g_{E+l} - g_{E-l}]}\cdot$$
$$\cdot\,[\delta(\boldsymbol{k} - \boldsymbol{k}_0) + \lambda^2 W[D_{E+l}(\boldsymbol{k}_0) - D_{E-l}(\boldsymbol{k}_0)]\,(2l)^{-1}]. \quad (3.11)$$

The asymptotic value of this expression at $t = +\infty$ is immediately obtained as the residue of the pole at $l = 0$. It is

$$P_E(\infty|\boldsymbol{k}\boldsymbol{k}_0) = \frac{iW}{2\pi}\,\frac{D_{E-i0}(\boldsymbol{k}) - D_{E+i0}(\boldsymbol{k})}{g_{E-i0} - g_{E+i0}}\,[D_{E-i0}(\boldsymbol{k}_0) - D_{E+i0}(\boldsymbol{k}_0)]. \quad (3.12)$$

Using (3.5) and the definition

$$\Delta_E(\boldsymbol{k}) = (2\pi i)^{-1}[D_{E+i0}(\boldsymbol{k}) - D_{E-i0}(\boldsymbol{k})],$$

this expression can be written

$$P_E(\infty|\boldsymbol{k}\boldsymbol{k}_0) = [\int \Delta_E(\boldsymbol{k}')\,\mathrm{d}\boldsymbol{k}']^{-1}\,\Delta_E(\boldsymbol{k})\,\Delta_E(\boldsymbol{k}_0), \quad (3.13)$$

in agreement with the corresponding result of the general theory (eqs. (7.6) and (7.7) of S'). As shown in S' this result corresponds to the establishment of microcanonical equilibrium (see S', pp. 475 and 476).

To study the behaviour of $P_E(t|\boldsymbol{k}\boldsymbol{k}_0)$ for finite times one needs an explicit expression of g_l, which would require solving the transcendental equation (3.7). We here avoid this difficult task and replace it by an (incomplete) investigation of the general behaviour of g_l in the complex l-plane. Therefore we examine the function $f(Z)$ of the complex variable Z defined by

$$f(Z) = 4\pi W\int_0^a \frac{k^2\,\mathrm{d}k}{k^2 - Z} \quad (3.14)$$

(we put $\varepsilon_{\boldsymbol{k}} = \boldsymbol{k}^2$, corresponding to a mass $\frac{1}{2}$ of the electron). This function has a square root branch point at $Z = 0$ and a logarithmic branch point at $Z = a^2$. If we put in (3.14) $Z = l + \lambda^2 g_l$, then (3.7) implies $f(Z) = g_l$. This gives us the relation between l and Z

$$l = Z - \lambda^2 f(Z), \quad (3.15)$$

from which we can find Z as a function $Z(l)$ of l. Knowing $Z(l)$, we shall have

$$g_l = f(Z(l)). \quad (3.16)$$

From these relations it is possible to study the behaviour of g_l as a function of l. The singularities of g_l will be situated in points l' such that $Z(l)$ becomes singular at $l = l'$, or such that $f(Z)$ behaves singularly at $Z = Z(l')$. The latter points correspond to $Z = 0$ and $Z = a^2$. The corresponding l' values are $-4\pi\lambda^2 Wa$ and ∞. One can show that g_l is regular in $l' = -4\pi\lambda^2 Wa$.

The singularities of $Z(l)$ must be obtained by solving the equation

$$\frac{\mathrm{d}l}{\mathrm{d}Z} = 1 - 4\pi\lambda^2 W \int_0^a \frac{k^2\,\mathrm{d}k}{(k^2 - Z)^2} = 0. \tag{3.17}$$

This equation has two roots on the real Z-axis: one for some value of $Z < 0$, with corresponding value of $l' = l_1$, $0 > l_1 > -4\pi\lambda^2 W a$, and one for a $Z > a^2$ with corresponding value of $l' = l_2$, $l_2 > a^2$. In the vicinity of l_1 and l_2, $Z(l)$ behaves like $(l - l_i)^{\frac{1}{2}}$, $i = 1,2$. Because $f(Z)$ is analytic and $\mathrm{d}f(Z)/\mathrm{d}Z$ not vanishing in these points, the corresponding singularities of g_l are fully characterized by those of $Z(l)$. It may further be proved that (3.17) has no roots for complex values of Z. Consequently g_l is analytic in the l-plane cut from l_1 to l_2 (see fig. 1) and has the latter points as square root branch points. The analytic continuation of g_l across the cut could be studied in detail. We shall not do so here and limit ourselves to the continuation obtained when Z describes the whole complex plane. Clearly this continuation of g_l has no new singularities.

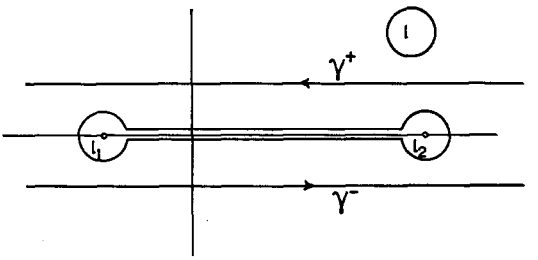

Fig. 1. Cut in the l-plane for g_l and original contour for $P_E(t|\boldsymbol{k}\boldsymbol{k}_0)$.

We now return to $P_E(t\,|\,\boldsymbol{k}\boldsymbol{k}_0)$, given by (3.11). Using (3.8) this expression may be written as

$$P_E(t\,|\,\boldsymbol{k}\boldsymbol{k}_0) = (2\pi^2)^{-1} \int_\gamma \mathrm{d}l \exp(2ilt)\, D_{E+l}(\boldsymbol{k})\, D_{E-l}(\boldsymbol{k}) \cdot$$
$$\cdot\, [\delta(\boldsymbol{k} - \boldsymbol{k}_0) + (2l)^{-1} \lambda^2 W [D_{E+l}(\boldsymbol{k}_0) - D_{E-l}(\boldsymbol{k}_0)]]. \tag{3.18}$$

The contour γ is composed of γ^+ and γ^- (see fig. 1). If we suppose t positive (as in (3.11)), γ^+ does not contribute; so we are left with γ^-. To evaluate this contour integration we continue g_l through the cut l_1, l_2 into the upper half plane. $D_l(\boldsymbol{k})$ and $D_l(\boldsymbol{k}_0)$ are there found to have each a pole at points $p_{\boldsymbol{k}}$ and $p_{\boldsymbol{k}_0}$ which we shall determine presently. The value of $P_E(t\,|\,\boldsymbol{k}\boldsymbol{k}_0)$ will then be calculated as if these poles were the only singularities of the D_l functions. We thereby neglect the contribution of all further singularities, especially of the branch points l_1, l_2. These further contributions, being of a completely different analytical form, do not modify the qualitative conclusions we shall reach concerning the time evolution of $P(t\,|\,\boldsymbol{k}\boldsymbol{k}_0)$.

The pole p_k of $D_l(\boldsymbol{k})$ may be found by requiring that

$$k^2 - p_k - \lambda^2 g_{p_k} = 0 \tag{3.19}$$

We now replace g_{p_k} by (3.7) for $l = p_k$. We get

$$p_k - k^2 - 4\pi\lambda^2 W \int_0^a \frac{k'^2\,\mathrm{d}k'}{k'^2 - p_k - \lambda^2 g_{p_k}} = k^2 - 4\pi\lambda^2 W \int_0^a \frac{k'^2\,\mathrm{d}k'}{k'^2 - k^2}, \tag{3.20}$$

where the integration over k' must be taken along the contour shown in

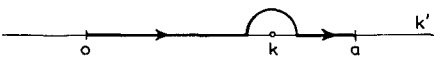

Fig. 2. Contour for the k'-integration in (3.20).

fig. 2 because l has been continued from lower to upper half of the l-plane. (3.20) can also be written

$$p_k = k^2 + 2\pi^2 i\lambda^2 W k - 4\pi\lambda^2 W\,\mathrm{P}\int_0^a \frac{k'^2\,\mathrm{d}k'}{k'^2 - k^2} \tag{3.21}$$

where P denotes the principal value of the integral. From (3.21) we deduce

$$p_k = k^2 - 4\pi W\lambda^2 a + 2\pi\lambda^2 W k \ln\frac{a+k}{a-k} + 2\pi^2 i\lambda^2 W k. \tag{3.22}$$

By the same method we can also find the residue N_k of $D_l(\boldsymbol{k})$ in p_k. The residue is given by

$$N_k^{-1} = \left(1 + \lambda^2 \frac{\mathrm{d}g_l}{\mathrm{d}l}\right)_{l=p_k}. \tag{3.23}$$

Now

$$g_l = 4\pi W \int_0^a \frac{k'^2\,\mathrm{d}k}{k'^2 - l - \lambda^2 g_l}. \tag{3.24}$$

Differentiating with respect to l gives us

$$\frac{\mathrm{d}g_l}{\mathrm{d}l} = 4\pi W \int_0^a \frac{k'^2\,\mathrm{d}k'}{(k'^2 - l - \lambda^2 g_l)^2}\left(1 + \lambda^2 \frac{\mathrm{d}g_l}{\mathrm{d}l}\right).$$

We calculate this expression in the pole p_k by the same method used to find p_k. The result is easily obtained:

$$\left(\frac{\mathrm{d}g_l}{\mathrm{d}l}\right)_{l=p_k} = \frac{2\pi W\left(\frac{1}{2}\ln\frac{a-k}{a+k} - \frac{ak}{a^2-k^2} - \pi i\right)}{k - \lambda^2\,2\pi W\left[\frac{1}{2}\ln\frac{a-k}{a+k} - \frac{ak}{a^2-k^2} - \pi i\right]} \tag{3.25}$$

and we find N_k by (3.23). We see that for a and $k \to \infty$, $N_k \to 1$; for small k, $N_k^{-1} \to 0$ (note that an electron with $k = 0$ has no dissipative properties).

In our calculation of $P_E(t\,|\,\boldsymbol{k}\boldsymbol{k}_0)$ we approximate N_k by 1. This is consistent with our approximation of considering p_k as the only singularity

of $D_l(\boldsymbol{k})$ in our evaluation of (3.18) by deformation of γ^-. We thus write approximately for $D_l(\boldsymbol{k})$

$$D_l(\boldsymbol{k}) = (p_{\boldsymbol{k}} - l)^{-1}. \tag{3.26}$$

It is convenient to abbreviate $p_{\boldsymbol{k}}$ as

$$p_{\boldsymbol{k}} = \bar{\varepsilon}_{\boldsymbol{k}} + i\gamma_{\boldsymbol{k}},\ \gamma_{\boldsymbol{k}} > 0 \tag{3.27}$$

where the real quantity $\bar{\varepsilon}_{\boldsymbol{k}}$ is the perturbed electron energy. (3.26) then gives

$$D_{E+l}(\boldsymbol{k}) = (\bar{\varepsilon}_{\boldsymbol{k}} + i\gamma_{\boldsymbol{k}} - E - l)^{-1},\ D_{E-l}(\boldsymbol{k}) = (\bar{\varepsilon}_{\boldsymbol{k}} - i\gamma_{\boldsymbol{k}} - E + l)^{-1}.$$

Using these expressions and similar ones for $\boldsymbol{k}_0$ we obtain the following approximate result for (3.18)

$$\begin{aligned}
P_E(t\,|\,\boldsymbol{k}\boldsymbol{k}_0) - P_E(\infty\,|\,\boldsymbol{k}\boldsymbol{k}_0) = &-\frac{i}{\pi}\exp\left[2it(\bar{\varepsilon}_{\boldsymbol{k}} - E + i\gamma_{\boldsymbol{k}})\right]\left[2(\bar{\varepsilon}_{\boldsymbol{k}} - E)\right]^{-1}\cdot \\
&\cdot\{\delta(\boldsymbol{k} - \boldsymbol{k}_0) + \lambda^2 W\left[2(\bar{\varepsilon}_{\boldsymbol{k}} - E + i\gamma_{\boldsymbol{k}})\right]^{-1}\cdot \\
&\cdot\left[(\bar{\varepsilon}_{\boldsymbol{k}_0} - \bar{\varepsilon}_{\boldsymbol{k}} - i\gamma_{\boldsymbol{k}} + i\gamma_{\boldsymbol{k}_0})^{-1} - (\bar{\varepsilon}_{\boldsymbol{k}_0} + \bar{\varepsilon}_{\boldsymbol{k}} - 2E + i\gamma_{\boldsymbol{k}} - i\gamma_{\boldsymbol{k}_0})^{-1}\right]\} + \\
&+\frac{i}{\pi}\exp[2it(E - \bar{\varepsilon}_{\boldsymbol{k}} + i\gamma_{\boldsymbol{k}})][2(\bar{\varepsilon}_{\boldsymbol{k}} - E)]^{-1}\cdot \\
&\cdot\{\delta(\boldsymbol{k} - \boldsymbol{k}_0) + \lambda^2 W[2(E - \bar{\varepsilon}_{\boldsymbol{k}} + i\gamma_{\boldsymbol{k}})]^{-1}\cdot \\
&\cdot\left[(\bar{\varepsilon}_{\boldsymbol{k}_0} + \bar{\varepsilon}_{\boldsymbol{k}} - 2E - i\gamma_{\boldsymbol{k}} + i\gamma_{\boldsymbol{k}_0})^{-1} - (\bar{\varepsilon}_{\boldsymbol{k}_0} - \bar{\varepsilon}_{\boldsymbol{k}} + i\gamma_{\boldsymbol{k}} - i\gamma_{\boldsymbol{k}_0})^{-1}\right]\} - \\
&-\frac{i\lambda^2 W}{2\pi}\exp\left[2it(\bar{\varepsilon}_{\boldsymbol{k}_0} - E + i\gamma_{\boldsymbol{k}_0})\right]\cdot \\
&\cdot\left[(\bar{\varepsilon}_{\boldsymbol{k}} - \bar{\varepsilon}_{\boldsymbol{k}_0} - i\gamma_{\boldsymbol{k}_0} + i\gamma_{\boldsymbol{k}})(\bar{\varepsilon}_{\boldsymbol{k}} + \bar{\varepsilon}_{\boldsymbol{k}_0} - 2E + i\gamma_{\boldsymbol{k}_0} - i\gamma_{\boldsymbol{k}})(\bar{\varepsilon}_{\boldsymbol{k}_0} - E + i\gamma_{\boldsymbol{k}_0})\right]^{-1} - \\
&-i\frac{\lambda^2 W}{2\pi}\exp\left[2it(E - \bar{\varepsilon}_{\boldsymbol{k}_0} + i\gamma_{\boldsymbol{k}_0})\right]\cdot \\
&\cdot\left[(\bar{\varepsilon}_{\boldsymbol{k}} + \bar{\varepsilon}_{\boldsymbol{k}_0} - 2E - i\gamma_{\boldsymbol{k}_0} + i\gamma_{\boldsymbol{k}})(\bar{\varepsilon}_{\boldsymbol{k}} - \bar{\varepsilon}_{\boldsymbol{k}_0} + i\gamma_{\boldsymbol{k}_0} - i\gamma_{\boldsymbol{k}})(E - \bar{\varepsilon}_{\boldsymbol{k}_0} + i\gamma_{\boldsymbol{k}_0})\right]^{-1}.
\end{aligned} \tag{3.28}$$

For $t = 0$, $P_E(t\,|\,\boldsymbol{k}\boldsymbol{k}_0)$ should be zero. This can be verified on (3.28) if $P_E(\infty\,|\,\boldsymbol{k}\boldsymbol{k}_0)$ is calculated from (3.18) with $D_l(\boldsymbol{k})$ replaced by (3.26). We now calculate the transition probability $P(t\,|\,\boldsymbol{k}\boldsymbol{k}_0)$ itself by integrating over E according to (2.12). This is done by contour integration for the second part of (3.28) (the one not involving $\delta(\boldsymbol{k} - \boldsymbol{k}_0)$). While the total function is seen to be regular in $E = \bar{\varepsilon}_{\boldsymbol{k}}$ it is convenient to integrate each term around this point. The following result is obtained

$$\begin{aligned}
P(t\,|\,\boldsymbol{k}\boldsymbol{k}_0) - P(\infty\,|\,\boldsymbol{k}\boldsymbol{k}_0) = &\exp(-2\gamma_{\boldsymbol{k}}t)\,\delta(\boldsymbol{k} - \boldsymbol{k}_0) - \\
&-\lambda^2 W\exp[it(\bar{\varepsilon}_{\boldsymbol{k}} - \bar{\varepsilon}_{\boldsymbol{k}_0})]\exp[-(\gamma_{\boldsymbol{k}} + \gamma_{\boldsymbol{k}_0})t]\cdot \\
&\cdot\left[\bar{\varepsilon}_{\boldsymbol{k}} - \bar{\varepsilon}_{\boldsymbol{k}_0} - i\gamma_{\boldsymbol{k}} + i\gamma_{\boldsymbol{k}_0}\right]^{-1}\left[\bar{\varepsilon}_{\boldsymbol{k}} - \bar{\varepsilon}_{\boldsymbol{k}_0} + i\gamma_{\boldsymbol{k}} + i\gamma_{\boldsymbol{k}_0}\right]^{-1} + \\
&+\lambda^2 W\exp[it(\bar{\varepsilon}_{\boldsymbol{k}_0} - \bar{\varepsilon}_{\boldsymbol{k}})]\exp[-(\gamma_{\boldsymbol{k}} + \gamma_{\boldsymbol{k}_0})t]\cdot \\
&\cdot\left[\bar{\varepsilon}_{\boldsymbol{k}} - \bar{\varepsilon}_{\boldsymbol{k}_0} + i\gamma_{\boldsymbol{k}} - i\gamma_{\boldsymbol{k}_0}\right]^{-1}\left[\bar{\varepsilon}_{\boldsymbol{k}_0} - \bar{\varepsilon}_{\boldsymbol{k}} + i\gamma_{\boldsymbol{k}} + i\gamma_{\boldsymbol{k}_0}\right]^{-1} + \\
&+\exp(-2\gamma_{\boldsymbol{k}}t)\frac{\lambda^2 W}{2i\gamma_{\boldsymbol{k}}}\left[(\bar{\varepsilon}_{\boldsymbol{k}_0} - \bar{\varepsilon}_{\boldsymbol{k}} - i\gamma_{\boldsymbol{k}} + i\gamma_{\boldsymbol{k}_0})^{-1} - (\bar{\varepsilon}_{\boldsymbol{k}_0} - \bar{\varepsilon}_{\boldsymbol{k}} + i\gamma_{\boldsymbol{k}} - i\gamma_{\boldsymbol{k}_0})^{-1}\right].
\end{aligned} \tag{3.29}$$

Writing this out in its explicit real form, one gets:

$$P(t\,|\,\boldsymbol{k}\boldsymbol{k}_0) - P(\infty\,|\,\boldsymbol{k}\boldsymbol{k}_0) = \exp(-2\gamma_{\boldsymbol{k}}t)\,\delta(\boldsymbol{k}-\boldsymbol{k}_0) -$$
$$-2\lambda^2 W \exp[-(\gamma_{\boldsymbol{k}}+\gamma_{\boldsymbol{k}_0})t]\{[(\bar{\varepsilon}_{\boldsymbol{k}}-\bar{\varepsilon}_{\boldsymbol{k}_0})^2+(\gamma_{\boldsymbol{k}}-\gamma_{\boldsymbol{k}_0})^2][(\bar{\varepsilon}_{\boldsymbol{k}}-\bar{\varepsilon}_{\boldsymbol{k}_0})^2+(\gamma_{\boldsymbol{k}}+\gamma_{\boldsymbol{k}_0})^2]\}^{-1}\cdot$$
$$\cdot\{[(\bar{\varepsilon}_{\boldsymbol{k}}-\bar{\varepsilon}_{\boldsymbol{k}_0})^2+(\gamma_{\boldsymbol{k}}{}^2-\gamma_{\boldsymbol{k}_0}{}^2)]\cos[(\bar{\varepsilon}_{\boldsymbol{k}}-\bar{\varepsilon}_{\boldsymbol{k}_0})t]+2\gamma_{\boldsymbol{k}_0}(\bar{\varepsilon}_{\boldsymbol{k}}-\bar{\varepsilon}_{\boldsymbol{k}_0})\sin[(\bar{\varepsilon}_{\boldsymbol{k}}-\bar{\varepsilon}_{\boldsymbol{k}_0})t]\}+$$
$$+\frac{\lambda^2 W}{\gamma_{\boldsymbol{k}}}\exp(-2\gamma_{\boldsymbol{k}}t)(\gamma_{\boldsymbol{k}}-\gamma_{\boldsymbol{k}_0})[(\bar{\varepsilon}_{\boldsymbol{k}}-\bar{\varepsilon}_{\boldsymbol{k}_0})^2+(\gamma_{\boldsymbol{k}}-\gamma_{\boldsymbol{k}_0})^2]^{-1}. \tag{3.30}$$

The value of $P(\infty\,|\,\boldsymbol{k}\boldsymbol{k}_0)$ in our approximation turns out to be

$$P(\infty\,|\,\boldsymbol{k}\boldsymbol{k}_0) = \frac{\lambda^2 W}{\gamma_{\boldsymbol{k}}}\,\frac{\gamma_{\boldsymbol{k}}+\gamma_{\boldsymbol{k}_0}}{[(\bar{\varepsilon}_{\boldsymbol{k}}-\bar{\varepsilon}_{\boldsymbol{k}_0})^2+(\gamma_{\boldsymbol{k}}+\gamma_{\boldsymbol{k}_0})^2]}\,. \tag{3.31}$$

It is interesting to compare (3.30) with the corresponding expression obtained in the limit of weak coupling. For t of order λ^{-2} it is

$$P(t\,|\,\boldsymbol{k}\boldsymbol{k}_0) - P(\infty\,|\,\boldsymbol{k}\boldsymbol{k}_0) =$$
$$= \exp(-2\gamma_{\boldsymbol{k}}t)\,\delta(\boldsymbol{k}-\boldsymbol{k}_0) - \frac{\pi\lambda^2 W}{\gamma_{\boldsymbol{k}}}\exp(-2\gamma_{\boldsymbol{k}}t)\,\delta(\varepsilon_{\boldsymbol{k}}-\varepsilon_{\boldsymbol{k}_0}), \tag{3.32}$$

which is the solution of the Pauli master equation in the simple situation treated here. The main difference between eqs. (3.30) and (3.32) is the occurrence of oscillating terms in the former. While the simplicity of (3.30) (in particular the absence of terms decreasing as a power of t) is of course due to the approximations (3.2) and (3.26), we expect that the occurrence of damped oscillations in $P(t\,|\,\boldsymbol{k}\boldsymbol{k}_0)$ will be a general feature of the transition probability when calculated to higher order in the interaction. From the behaviour of the simple case treated here this feature appears to be the most prominent observable consequence of the non-markovian property we have seen to hold for the time evolution of the coarse grained probability (i.e. of the memory effect contained in the generalized master equation (2.13)).

In an actual system this effect would manifest itself for example when an external electric field which has been acting long enough to give a stationary current is suddenly turned off: the current while dying out would then perform some damped oscillations. This effect, however, would only appear when the electron-lattice interaction is strong, i.e. when the relaxation time is short, so that the times involved may be too short for actual observation in metals or semi-conductors. Other dissipative systems involving slower time scales, like for example spin systems, might present more favorable conditions. Let us quote in that respect the nuclear spin system of a crystal. Although the present theory is not directly applicable to this situation, due to the discreteness of the quantum numbers, it is possible to develop a theory based upon the same principles [3]). Actual observations of nuclear spin relaxation as made by Lowe and Norberg [4]) have revealed oscillatory behaviour.

4. *An electron in a phonon gas.* We consider in the present section a slightly more complicated situation: one conduction electron in a vibrating harmonic lattice, i.e. in a phonon gas. This system has been considered previously as an illustration of the general formalism, with special attention to the weak coupling case: a detailed derivation has been given for the lowest order master equation describing the evolution of the electron-phonon system, and for the resulting Boltzmann equation which describes the time evolution of the electron alone [5]. We here consider the same system to general order in the electron-phonon interaction and wish to derive from the generalized master equation a generalized Boltzmann equation for the time evolution of the electron alone. When the phonon energies are neglected compared to the electron energy, this equation has the form (2.13) with α_0, α, α' replaced by the electron wave vectors. This is exactly the type of equation treated in the foregoing section.

We consider a crystal of volume Ω. The harmonic lattice vibrations are described in terms of phonons, characterized by their wave vector $\boldsymbol{q}$ (we neglect the polarization). The states of the conduction electron are labelled by its momentum $\boldsymbol{k}$, the spin being neglected. We denote the phonon energy by $\omega_{\boldsymbol{q}}$ and the electron energy by $\varepsilon_{\boldsymbol{k}}$. The Hamiltonian $H' = H + \lambda V$ has the form

$$H = \Sigma_{\boldsymbol{q}} \omega_{\boldsymbol{q}} a^*_{\boldsymbol{q}} a_{\boldsymbol{q}} + \Sigma_{\boldsymbol{k}} \varepsilon_{\boldsymbol{k}} \alpha^*_{\boldsymbol{k}} \alpha_{\boldsymbol{k}}, \tag{4.1}$$

$$\lambda V = \lambda \left(\frac{8\pi^3}{\Omega}\right)^{\frac{1}{2}} \Sigma_{\boldsymbol{kq}} \left[f_{\boldsymbol{kq}} a^*_{\boldsymbol{q}} \alpha^*_{\boldsymbol{k}-\boldsymbol{q}} \alpha_{\boldsymbol{k}} + f^*_{\boldsymbol{kq}} a_{\boldsymbol{q}} \alpha^*_{\boldsymbol{k}} \alpha_{\boldsymbol{k}-\boldsymbol{q}}\right], \tag{4.2}$$

with the usual commutation and anticommutation rules for the $a_{\boldsymbol{q}}$, $a^*_{\boldsymbol{q}}$ and $\alpha_{\boldsymbol{k}}$, $\alpha^*_{\boldsymbol{k}}$. Under periodic boundary conditions the components of $\boldsymbol{q}$ and $\boldsymbol{k}$ run over integral multiples of $2\pi\Omega^{-\frac{1}{3}}$. The sum over $\boldsymbol{q}$ is restricted to the first Brillouin zone. We extend the sum over $\boldsymbol{k}$ to the whole $\boldsymbol{k}$-space, thus neglecting the band structure of the electron. In the limit of an infinite crystal the sum $8\pi^3\Omega^{-1}\Sigma_{\boldsymbol{q}}$ can be replaced by $\int d\boldsymbol{q}$ and $(\Omega/8\pi^3)\,\delta_{\boldsymbol{q},\boldsymbol{q}'}$ becomes the three dimensional delta function $\delta(\boldsymbol{q} - \boldsymbol{q}')$. Because we limit ourselves to states with one electron, the basic states can be written

$$|\alpha\rangle = (\Omega/8\pi^3)^{N+1}\, \alpha^*_{\boldsymbol{k}} a^*_{\boldsymbol{q}_1} \ldots a^*_{\boldsymbol{q}_N} |0\rangle, \tag{4.3}$$

where $|0\rangle$ is the no electron, no phonon state. These states have the required normalization (2.2) for $\Omega \to \infty$. We actually are interested in states (4.3) where N is of the same order as Ω, so that there is a finite phonon density in ordinary space. For such states we define two distribution functions of the phonons in $\boldsymbol{q}$-space, $n_{\boldsymbol{q}}$ and $\tilde{n}_{\boldsymbol{q}}$. The former $n_{\boldsymbol{q}}$ is simply the occupation number of the phonon state $\boldsymbol{q}$ in the state α; it has integral values and will be called the fine grained distribution. $\tilde{n}_{\boldsymbol{q}}$ is the coarse-grained distribution deduced from $n_{\boldsymbol{q}}$ by averaging over a small but finite volume element $\Delta_{\boldsymbol{q}}$ in $\boldsymbol{q}$-space

$$(\Omega/8\pi^3)\, \tilde{n}_{\boldsymbol{q}} \Delta\boldsymbol{q} = \Sigma_{\Delta\boldsymbol{q}}\, n_{\boldsymbol{q}}, \tag{4.4}$$

where the sum extends over all $\boldsymbol{q}$ in $\Delta\boldsymbol{q}$. We shall assume $\tilde{n}_{\boldsymbol{q}}$ to be smooth in $\boldsymbol{q}$. In the limit of an infinite system this function will remain unchanged under creation or destruction of any finite number of phonons. Consequently for any finite time and any finite order in the electron-phonon interactions $P_E(t\,|\,\alpha'\alpha)$ and $w_E(t\,|\,\alpha'\alpha)$ differ from zero only when the state α' has the same coarse grained distribution as the state α, and in the generalized master equation (2.13) we can assume that all states α', α, α_0 have the same coarse grained distribution $\tilde{n}_{\boldsymbol{q}}$.

We write down the master equation (2.13) for this specific system:

$$\frac{\mathrm{d}P_E(t\,|\,\alpha\alpha_0)}{\mathrm{d}t} = \delta(\alpha - \alpha_0)\, f_E(t\,|\,\alpha) +$$

$$+ 2\pi\lambda^2 \int_0^t \mathrm{d}t' \left[\sum_{i=0}^{\infty} \sum_{j=0}^{\infty} \int \mathrm{d}\boldsymbol{k}' \prod_{\rho=1}^{i} \mathrm{d}\boldsymbol{q}_\rho \prod_{\sigma=1}^{j} \mathrm{d}\boldsymbol{q}_\sigma' w_E(t-t'\,|\,\alpha\alpha') P_E(t'\,|\,\alpha'\alpha_0) \right] -$$

$$- 2\pi\lambda^2 \int_0^t \mathrm{d}t' \left[\sum_{i=0}^{\infty} \sum_{j=0}^{\infty} \int \mathrm{d}\boldsymbol{k}' \prod_{\rho=1}^{i} \mathrm{d}\boldsymbol{q}_\rho \prod_{\sigma=1}^{j} \mathrm{d}\boldsymbol{q}_\sigma' w_E(t-t'\,|\,\alpha'\alpha) \right] P_E(t'\,|\,\alpha\alpha_0). \quad (4.5)$$

In this equation $\boldsymbol{k}'$ is the electron momentum in α'. The phonon distribution in α' differs from that in α by the fact that phonons $\boldsymbol{q}_1, \ldots \boldsymbol{q}_i$ have been removed and phonons $\boldsymbol{q}_1', \ldots \boldsymbol{q}_j'$ added. From (4.5) it is possible to derive an equation describing the evolution of the electron alone. We first remark that the eigenvalues $D_l(\alpha)$, $G_l(\alpha)$ of the operators (2.18), (2.19) depend in a very special way on the phonon distribution in the state $|\alpha\rangle$. $D_l(\alpha)$, $G_l(\alpha)$ are actually functions of $\boldsymbol{k}$ (the electron momentum in α), the coarse graine distribution $\tilde{n}_{\boldsymbol{q}}$ and the number

$$\bar{l} = l - \textstyle\sum_{\boldsymbol{q}} n_{\boldsymbol{q}} \omega_{\boldsymbol{q}}, \quad (4.6)$$

where $n_{\boldsymbol{q}}$ is the fine grained distribution of the phonons in $|\alpha\rangle$. As is readily checked by calculating $G_l(\alpha)$ to some low order, $\bar{l}$ is the only combination through which the fine grained distribution enters $G_l(\alpha)$ and $D_l(\alpha)$. We write accordingly

$$D_l(\alpha) = \bar{D}_{\bar{l}}(\boldsymbol{k}). \quad (4.7)$$

In this and later equations the dependence on $\tilde{n}_{\boldsymbol{q}}$ is left out because, as mentioned above, we can assume $\tilde{n}_{\boldsymbol{q}}$ to be the same for all states to be considered. Similarly the function $\tilde{W}_{ll'}(\alpha'\alpha)$ turns out to depend only on $\boldsymbol{k}$, $\boldsymbol{k}'$ (the electron momenta in α and α'), $\bar{l}$ (as defined in (4.6)), $l' - l$, and the phonons $\boldsymbol{q}_1 \ldots, \boldsymbol{q}_i$, $\boldsymbol{q}_1' \ldots, \boldsymbol{q}_j'$ which, as defined above, make the difference between the phonon distribution in α and α'. Thus

$$\tilde{W}_{ll'}(\alpha'\alpha) = \overline{W}_{\bar{l},l-l'}(\boldsymbol{k}'\boldsymbol{k}, \boldsymbol{q}_1' \ldots \boldsymbol{q}_j', \boldsymbol{q}_1 \ldots \boldsymbol{q}_i). \quad (4.8)$$

Momentum conservation actually implies that the function (4.8) contains the factor

$$\delta(\boldsymbol{k}' + \boldsymbol{q}_1' + \ldots + \boldsymbol{q}_j' - \boldsymbol{k} - \boldsymbol{q}_1 \ldots - \boldsymbol{q}_i). \quad (4.9)$$

Inserting (4.7) in the definition (2.26) we find

$$f_E(t\,|\,\alpha) = \bar{f}_{\bar{E}}(t\,|\,\boldsymbol{k}) \tag{4.10}$$

with

$$\bar{E} = E - \Sigma_{\boldsymbol{q}}\, n_{\boldsymbol{q}}\omega_{\boldsymbol{q}}. \tag{4.11}$$

Similarly insertion of (4.8) into (2.25) gives

$$w_E(t\,|\,\alpha'\alpha) = \bar{w}_{\bar{E}}(t\,|\,\boldsymbol{k}'\boldsymbol{k},\, \boldsymbol{q}_1' \ldots \boldsymbol{q}_j',\, \boldsymbol{q}_1 \ldots \boldsymbol{q}_i). \tag{4.12}$$

Also the latter function contains (4.9) as the momentum conservation factor.

W now introduce the partial transition probability $\bar{P}_\varepsilon(t\,|\,\boldsymbol{k}\boldsymbol{k}_0)$ for the electron alone, which will be shown to obey a generalized Boltzmann equation. Let

$$|\varphi_0\rangle = \int |\alpha_0\rangle\, \mathrm{d}\alpha_0\, c(\alpha_0)$$

be the wave function of the electron-phonon system at time $t = 0$ and assume as before that all states for which $c(\alpha_0) \neq 0$ have the same coarse grained phonon distribution $\tilde{n}_{\boldsymbol{q}}$. Define

$$\bar{P}_\varepsilon(t\,|\,\boldsymbol{k}\boldsymbol{k}_0) = [p(\boldsymbol{k}_0)]^{-1} \cdot \int_{(\alpha)} \mathrm{d}\alpha \int_{(\alpha_0)} \mathrm{d}\alpha_0\, P_{E(\varepsilon\alpha)}(t\,|\,\alpha\alpha_0)|c(\alpha_0)|^2, \tag{4.13}$$

$$p(\boldsymbol{k}_0) = \int_{(\alpha_0)} |c(\alpha_0)|^2\, \mathrm{d}\alpha_0, \tag{4.14}$$

where the integral in α runs over all states with electron momentum $\boldsymbol{k}$ and the two integrals in α_0 over all states with electron momentum $\boldsymbol{k}_0$. $P_{E(\varepsilon\alpha)}|(t|\alpha\alpha_0)$ is the same quantity as in (4.5) except that the suffix E is replaced by

$$E(\varepsilon\alpha) = \varepsilon + \Sigma_{\boldsymbol{q}}\, n_{\boldsymbol{q}}\omega_{\boldsymbol{q}} \tag{4.15}$$

$n_{\boldsymbol{q}}$ being the fine grained phonon distribution of α. Note that

$$E(\varepsilon\alpha) = E(\varepsilon'\alpha') \text{ with } \varepsilon' = \varepsilon + \omega_{\boldsymbol{q}_1} + \ldots + \omega_{\boldsymbol{q}_i} - \omega_{\boldsymbol{q}_1'} - \ldots - \omega_{\boldsymbol{q}_j'}. \tag{4.16}$$

Return now to the master equation (4.5). Replace E by $E(\varepsilon\alpha)$ everywhere except in $w_E(t - t'\,|\,\alpha, \alpha')\, P_E(t'\,|\,\alpha'\alpha_0)$ where it has to be replaced by the identical quantity $E(\varepsilon'\alpha')$. Using (4.10), (4.11), make the substitution

$$f_{E(\varepsilon,\alpha)}(t\,|\,\alpha) = \bar{f}_\varepsilon(t\,|\,\boldsymbol{k})$$

Similarly, with (4.11), (4.12) substitute

$$w_{E(\varepsilon\alpha)}(t - t'\,|\,\alpha'\alpha) = \bar{w}_\varepsilon(t - t'\,|\,\boldsymbol{k}'\boldsymbol{k},\, \boldsymbol{q}_1' \ldots \boldsymbol{q}_j',\, \boldsymbol{q}_1 \ldots \boldsymbol{q}_i)$$

$$w_{E(\varepsilon'\alpha')}(t - t'\,|\,\alpha\alpha') = \bar{w}_{\varepsilon'}(t - t'\,|\,\boldsymbol{k}\boldsymbol{k}',\, \boldsymbol{q}_1 \ldots \boldsymbol{q}_i,\, \boldsymbol{q}_1' \ldots \boldsymbol{q}_j').$$

Multiply both sides of (4.5) by $|c(\alpha_0)|^2/p(\boldsymbol{k}_0)$ and sum over all α_0 with electron monentum $\boldsymbol{k}_0$. Sum further both sides over all α with electron momentum $\boldsymbol{k}$; for fixed $\boldsymbol{q}_1, \ldots \boldsymbol{q}_i,\ \boldsymbol{q}_1' \ldots \boldsymbol{q}_j'$ the state α' then runs over all states with electron momentum

$$\boldsymbol{k}' = \boldsymbol{k} + \boldsymbol{q}_1 + \ldots + \boldsymbol{q}_i - \boldsymbol{q}_1' - \ldots - \boldsymbol{q}_j'.$$

Using (4.13), these summations amount to replacing $P_{E(\varepsilon\alpha)}(t\,|\,\alpha\alpha_0)$ by

$\bar{P}_\varepsilon(t\,|\,\boldsymbol{k}\boldsymbol{k}_0)$ and $P_{E(\varepsilon'\alpha')}(t'\,|\,\alpha'\alpha_0)$ by $\bar{P}_{\varepsilon'}(t'\,|\,\boldsymbol{k}'\boldsymbol{k}_0)$. The result is the following *generalized Boltzmann equation* for an electron in a phonon gas

$$\frac{\mathrm{d}}{\mathrm{d}t}\bar{P}_\varepsilon(t\,|\,\boldsymbol{k}\boldsymbol{k}_0) = \delta(\boldsymbol{k}-\boldsymbol{k}_0)\,\bar{f}_\varepsilon(t\,|\,\boldsymbol{k}) + \\ + 2\pi\lambda^2\int_0^t \mathrm{d}t' \sum_{i=0}^{\infty}\sum_{j=0}^{\infty}\int \mathrm{d}\boldsymbol{k}'\,\Pi_{\rho=1}^{i}\,\mathrm{d}\boldsymbol{q}_\rho\,\Pi_{\sigma=1}^{j}\,\mathrm{d}\boldsymbol{q}_\sigma' \cdot \\ \cdot\,\bar{w}_{\varepsilon'}(t-t'\,|\,\boldsymbol{k}\boldsymbol{k}',\,\boldsymbol{q}_1\ldots\boldsymbol{q}_i,\,\boldsymbol{q}_1'\ldots\boldsymbol{q}_j')\bar{P}_{\varepsilon'}(t'\,|\,\boldsymbol{k}'\boldsymbol{k}_0) - \\ - 2\pi\lambda^2\int_0^t \mathrm{d}t' \sum_{i=0}^{\infty}\sum_{j=0}^{\infty}\int \mathrm{d}\boldsymbol{k}'\,\Pi_{\rho=1}^{i}\,\mathrm{d}\boldsymbol{q}_\rho\,\Pi_{\sigma=1}^{j}\,\mathrm{d}\boldsymbol{q}_\sigma' \cdot \\ \cdot\,\bar{w}_\varepsilon(t-t'\,|\,\boldsymbol{k}'\boldsymbol{k},\,\boldsymbol{q}_1'\ldots\boldsymbol{q}_j',\,\boldsymbol{q}_1\ldots\boldsymbol{q}_i)\,\bar{P}_\varepsilon(t'\,|\,\boldsymbol{k}\boldsymbol{k}_0), \qquad (4.17)$$

where ε' is, as before, the following function of ε, $\boldsymbol{q}_\rho$ and $\boldsymbol{q}_\sigma'$

$$\varepsilon' = \varepsilon + \sum_{\rho=1}^{i}\omega_{\boldsymbol{q}_\rho} - \sum_{\sigma=1}^{j}\omega_{\boldsymbol{q}_\sigma'}. \qquad (4.18)$$

Eq. (4.17) may be simplified further if the phonon energies can be neglected with respect to the electron energy. ε' can then be identified with ε and we find

$$\frac{\mathrm{d}\bar{P}_\varepsilon(t\,|\,\boldsymbol{k}\boldsymbol{k}_0)}{\mathrm{d}t} = \delta(\boldsymbol{k}-\boldsymbol{k}_0)\,\bar{f}_\varepsilon(t\,|\,\boldsymbol{k}) + \\ + 2\pi\lambda^2\int_0^t \mathrm{d}t'\int \mathrm{d}\boldsymbol{k}' w_\varepsilon(t-t'\,|\,\boldsymbol{k}\boldsymbol{k}')\,\bar{P}_\varepsilon(t'\,|\,\boldsymbol{k}'\boldsymbol{k}_0) \\ - 2\pi\lambda^2\int_0^t \mathrm{d}t'\int \mathrm{d}\boldsymbol{k}' w_\varepsilon(t-t'\,|\,\boldsymbol{k}'\boldsymbol{k})\,\bar{P}_\varepsilon(t'\,|\,\boldsymbol{k}\boldsymbol{k}_0) \qquad (4.19)$$

with

$$w_\varepsilon(t-t'\,|\,\boldsymbol{k}\boldsymbol{k}') = \sum_{i=0}^{\infty}\sum_{j=0}^{\infty}\int \Pi_{\rho=1}^{i}\mathrm{d}\boldsymbol{q}_\rho\,\Pi_{\sigma=1}^{j}\mathrm{d}\boldsymbol{q}_\sigma' w_\varepsilon(t-t'\,|\,\boldsymbol{k}\boldsymbol{k}',\,\boldsymbol{q}_1\ldots\boldsymbol{q}_i,\,\boldsymbol{q}_1'\ldots\boldsymbol{q}_j'). \qquad (4.20)$$

Eq. (4.19) entirely agrees with the generalized Boltzmann equation for an electron in a system of random scattering centers, which is the case studied in the previous section. The approximate solution there obtained also illustrates the behaviour of an electron in a phonon gas under neglection of the phonon energies. It might be interesting to look for an approximate solution of equation (4.17) which incorporates these energies, but no attempt has been made in this direction.

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