man sogar gelegentlich nur noch 5% der ursprünglichen Zwillingszahl finden. Daraus kann man schließen – zu ähnlichen Folgerungen führten Schmelzpunktsbestimmungen an dünnen Schichten im Elektronenmikroskop –, daß der sich durch die Bestrahlung auf beiden Seiten der Metallschicht bildende Kohlefilm eine stabilisierende Wirkung ausübt und so das Verschwinden der Zwillinge erschwert.

Auch nach längerem Erhitzen in der Nähe des Schmelzpunktes des kompakten Metalles bleiben noch etwa $1 \cdot 10^{13} - 5 \cdot 10^{14}$ Strukturen pro cm^3 übrig, obwohl an manchen Stellen der Folie bei diesen Temperaturen bereits ein Absublimieren des Materials stattfindet. Dem Absublimieren geht keineswegs eine Umwandlung (Verschwinden des Zwillings) voraus; auch ein bevorzugter Abbau an Zwilling oder Matrix wurde nicht gefunden.

Bei allen drei Metallen wurden nach längerem Verweilen in der Nähe der Schmelztemperatur noch Zwillinge gefunden, die im Beugungsbild deutliche Zwillingsreflexe lieferten. Das Ergebnis von Bahadur u. a. [23], daß bei Temperaturen über 650 °C die Zusatzringe bei Gold verschwinden, kann deshalb nicht bestätigt werden.

4.2. Zum Vorgang der Umwandlung von Zwillingsorientierung in die (100)-Matrix-Orientierung

Da am Orte des Verschwindens der Zwillinge keine Dickenänderung der Folie beobachtet wird, muß das Unsichtbarwerden dieser Strukturen als Umwandlungsvorgang zu deuten sein. Wir nehmen also an, daß an diesen Stellen die Matrixorientierung energetisch günstiger liegt (wegen des Verschwindens der Zwillingsgrenzen), und sich deshalb der Zwilling in die andere spiegelbildliche Orientierungslage umlagert. Der Vergleich von bestrahlten und unbestrahlten Stellen gibt Hinweise darauf, daß die Umwandlung nicht im Inneren, sondern an der Ober- oder Unterseite der Schicht ihren Ausgang nimmt.

Die Bildungswahrscheinlichkeit für die Umwandlungskeime und die Umwandlungsgeschwindigkeit selbst nimmt mit höherer Temperatur zu.

Der Arbeitsgemeinschaft für Elektronenoptik e. V. und den Wirtschaftsministerien des Bundes und des Landes Baden-Württemberg ist für die Unterstützung der Untersuchungen zu danken.

Space-correlation Function Expression for the Real Part of the Electrical Conductivity

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(Z. Naturforschg. **20 a**, 1207—1212 [1965]; received 5 June 1965)

The real part of the frequency and wave-vector dependent conductivity is expressed in terms of single-particle and pair correlation functions starting from a generalized Kubo formula. The result is an analogon to Zwanzig's relation between the self-diffusion coefficient and the dynamical structure factor introduced by Van Hove in the theory of neutron scattering. As an application we calculate the real part of the mobility for the small polaron.

Recently, Baym [1] and Greene and Kohn [2] pointed out that the problem of electron-phonon interaction in solids and liquids can be completely described in terms of the dynamical structure factor

$$S(\boldsymbol{q},\omega) = \frac{1}{2\pi N_0}\int_{-\infty}^{+\infty} \mathrm{d}t\, e^{-i\omega t} \left\langle \sum_{j,l} \exp\{-i\,\boldsymbol{q}\cdot\boldsymbol{R}_j(0)\}\, \exp\{i\,\boldsymbol{q}\cdot\boldsymbol{R}_l(t)\}\right\rangle. \quad (1)$$

$\langle \ldots \rangle$ represents a thermal average at temperature T, $\boldsymbol{R}_l(t)$ is the Heisenberg operator for the position of the l-th ion at time t, N_0 the number of scattering centres and $\boldsymbol{q} = \boldsymbol{k} - \boldsymbol{k}'$ the difference of wave vectors in the initial and final electron states. The expression for the resistivity given in ref. [1] and [2] is valid in the Born approximation for the electron-phonon scattering.

On the other hand, the information about the dynamics of the ions contained in $S(\boldsymbol{q},\omega)$ may also be used to study certain transport properties of the

[1] G. Baym, Phys. Rev. **135**, A 1691 [1964].
[2] M. P. Greene and W. Kohn, Phys. Rev. **137**, A 513 [1965].

ions themselves (see ref. [3]). The most general relation between the dynamical structure factor and a generalized frequency and wave-vector dependent self-diffusion coefficient has been given in a short note by ZWANZIG [4]. His derivation consists in establishing the connection between the KUBO-formula for the real part of the diffusion coefficient in a system with arbitrary space-time variations, and the FOURIER transform of the space- and time-dependent pair correlation function defined in the integrand of (1). [Of course, in the case of inelastic neutron scattering – by which $S(\boldsymbol{q}, \omega)$ can be directly measured – the wave vector $\boldsymbol{q}$ corresponds to the momentum transfer of the neutrons and ω to the neutron energy.] The work of ZWANZIG suggests that it might be possible to express the KUBO-formula for the electrical resistivity in terms of a formal analogon to (1). According to the different physical problem, the position operators now belong to the various charge carriers and the variables $(\boldsymbol{q}, \omega)$ enter by considering a frequency- and wave vector-dependent driving electric field.

The aim of the present paper is to establish the relation between the real part of the electrical conductivity and the dynamical structure factor for the electrons. As an application, we have rederived the expression for the frequency-dependent mobility for the small polaron [5] in the limit $\boldsymbol{q} \to 0$, i. e. for an electric field constant in space. Our work benefits from many considerations already contained in the basic paper of KUBO [6].

General Formulation

We consider a system of unit volume, invariant under translation in space and time. The FOURIER transform of the linear, nonlocal OHM's law is then given by

$$\langle j_\alpha(\boldsymbol{q}, \omega) \rangle = \sigma_{\alpha\gamma}(\boldsymbol{q}, \omega)\, E_\gamma(\boldsymbol{q}, \omega), \quad (\alpha, \gamma = 1, 2, 3). \tag{2}$$

We start from the following expression for the α-*th* component of the average current density [6]

$$\langle j_\alpha(\boldsymbol{x}) \rangle = \lim_{s \to 0} \int_0^\infty \mathrm{d}t\, e^{-(i\omega+s)t} \int_0^\beta \mathrm{d}\lambda \int \mathrm{d}\boldsymbol{x}' \langle j_\gamma(\boldsymbol{x}', -t - i\hbar\lambda)\, j_\alpha(\boldsymbol{x}) \rangle\, E_\gamma(\boldsymbol{x}'), \tag{3}$$

which describes the linear response of the system to a gradually turned on external electric field with a time-dependence $e^{i\omega t}$. Let the electric field have only one FOURIER component

$$E_\gamma(\boldsymbol{x}) = \exp\{-i\,\boldsymbol{q}\cdot\boldsymbol{x}\}\, E_\gamma(\boldsymbol{q})$$

then the FOURIER transform of the average current density is given by

$$\langle j_\alpha(\boldsymbol{q}) \rangle = \lim_{s \to 0} \int_0^\infty \mathrm{d}t\, e^{-(i\omega+s)t} \int_0^\beta \mathrm{d}\lambda \langle j_\gamma(-\boldsymbol{q}, -t - i\hbar\lambda)\, j_\alpha(\boldsymbol{q}) \rangle\, E_\gamma(\boldsymbol{q}). \tag{4}$$

By comparison with the phenomenological equation (2) we have

$$\sigma_{\alpha\gamma}(\boldsymbol{q}, \omega) = \lim_{s \to 0} \int_0^\infty \mathrm{d}t\, e^{-(i\omega+s)t} \int_0^\beta \mathrm{d}\lambda \langle j_\gamma(-\boldsymbol{q}, -t - i\hbar\lambda)\, j_\alpha(\boldsymbol{q}) \rangle\,. \tag{5}$$

(For convenience we omit the adiabatic factor e^{-st} during the calculations until the final result is obtained.) The current-density and charge-density operators

$$\boldsymbol{j}(\boldsymbol{x}) = \tfrac{1}{2} e \sum_j \{\boldsymbol{v}_j\, \delta(\boldsymbol{x} - \boldsymbol{r}_j) + \delta(\boldsymbol{x} - \boldsymbol{r}_j)\, \boldsymbol{v}_j\}, \quad \varrho(\boldsymbol{x}) = e \sum_j \delta(\boldsymbol{x} - \boldsymbol{r}_j) \tag{6}$$

have the FOURIER transforms

$$\boldsymbol{j}(\boldsymbol{q}) = \tfrac{1}{2} e \sum_j \{\boldsymbol{v}_j \exp[i\,\boldsymbol{q}\cdot\boldsymbol{r}_j] + \exp[i\,\boldsymbol{q}\cdot\boldsymbol{r}_j]\, \boldsymbol{v}_j\}, \quad \varrho(\boldsymbol{q}) = e \sum_j \exp[i\,\boldsymbol{q}\cdot\boldsymbol{r}_j], \tag{7}$$

resp. The sum is over all charge carriers of charge e and particle velocity $\boldsymbol{v}_j$.

[3] P. SCHOFIELD in: Fluctuation, Relaxation and Resonance in Magnetic Systems, Scottish Universities' Summer School 1961, Oliver & Boyd, Edinburgh and London, p. 207.
[4] R. ZWANZIG, Phys. Rev. **133**, A 50 [1964].
[5] H. G. REIK, Solid State Comm. **1**, 67 [1963].
[6] R. KUBO, J. Phys. Soc. Japan **12**, 570 [1957], see also Lectures in Theoretical Physics, Boulder 1958, Interscience Publishers, Inc., New York 1959, Vol. I.

With the help of the equation of continuity

$$\dot{\varrho}\,(\boldsymbol{x},t) = -\operatorname{div}\boldsymbol{j}(\boldsymbol{x},t) = (1/i\hbar)\,[\varrho(\boldsymbol{x},t), H]\,,\quad \dot{\varrho}\,(\boldsymbol{q},t) = -i\,\boldsymbol{q}\cdot\boldsymbol{j}(\boldsymbol{q},t) \tag{8), (9}$$

the current density operators can be eliminated from (5) to yield the result

$$q_\alpha\, q_\gamma\, \sigma_{\alpha\gamma}(\boldsymbol{q},\omega) = \int_0^\infty \mathrm{d}t\, e^{-i\omega t} \int_0^\beta \mathrm{d}\lambda \langle\, \dot{\varrho}\,(-\boldsymbol{q}, -t - i\hbar\lambda)\, \dot{\varrho}\,(\boldsymbol{q})\,\rangle \tag{10}$$

or

$$q_\alpha\, q_\gamma\, \sigma_{\alpha\gamma}(\boldsymbol{q},\omega) = -e^2 \int_0^\infty \mathrm{d}t\, e^{-i\omega t}\, \frac{\partial^2}{\partial t^2} \int_0^\beta \mathrm{d}\lambda \,\langle \sum_{j,l} \exp[-i\,\boldsymbol{q}\cdot\boldsymbol{r}_j(-t-i\hbar\lambda)]\exp[i\,\boldsymbol{q}\cdot\boldsymbol{r}_l]\,\rangle. \tag{11}$$

From (10) to (11) we used the identity

$$\langle \dot{\varrho}\,(-\boldsymbol{q}, -t - i\hbar\lambda)\, \dot{\varrho}\,(\boldsymbol{q})\,\rangle = -\frac{\partial^2}{\partial t^2}\,\langle \varrho(-\boldsymbol{q}, -t - i\hbar\lambda)\, \varrho(\boldsymbol{q})\,\rangle$$

for the ensemble average of HEISENBERG operators.

From now on we consider only the real part of $q_\alpha\, q_\gamma\, \sigma_{\alpha\gamma}(\boldsymbol{q},\omega)$. We obtain

$$\begin{aligned} q_\alpha\, q_\gamma \operatorname{Re}\sigma_{\alpha\gamma}(\boldsymbol{q},\omega) &= \tfrac{1}{2}\, q_\alpha\, q_\gamma\, \{\sigma_{\alpha\gamma}(\boldsymbol{q},\omega) + \sigma^*_{\alpha\gamma}(\boldsymbol{q},\omega)\} \\ &= -\frac{e^2}{2} \int_{-\infty}^{+\infty} \mathrm{d}t\, e^{-i\omega t}\, \frac{\partial^2}{\partial t^2} \int_0^\beta \mathrm{d}\lambda\, \langle \sum_{j,l} \exp[-i\,\boldsymbol{q}\cdot\boldsymbol{r}_j(-t-i\hbar\lambda)]\, \exp[i\,\boldsymbol{q}\cdot\boldsymbol{r}_l]\,\rangle \end{aligned} \tag{12}$$

or, integrating by parts,

$$q_\alpha\, q_\gamma \operatorname{Re}\sigma_{\alpha\gamma}(\boldsymbol{q},\omega) = \frac{e^2\,\omega^2}{2} \int_{-\infty}^{+\infty} \mathrm{d}t\, e^{-i\omega t} \int_0^\beta \mathrm{d}\lambda\, \langle \sum_{j,l} \exp[-i\,\boldsymbol{q}\cdot\boldsymbol{r}_j(-t-i\hbar\lambda)]\, \exp[i\,\boldsymbol{q}\cdot\boldsymbol{r}_l]\,\rangle, \tag{13}$$

provided the correlation functions vanish at $t = \pm\infty$. If we take the thermal average of an operator A,

$$\langle A\rangle \equiv (1/Z)\,\operatorname{Tr}(\varrho\, A)$$

over a canonical ensemble, that is with an equilibrium density operator $\varrho_{\mathrm{T}} = \exp(-\beta H)$, the right hand side of (13) can be considerable simplified by using the following identity

$$\int_{-\infty}^{+\infty} \mathrm{d}t\, e^{-i\omega t} \int_0^\beta \mathrm{d}\lambda \langle A\, B(t + i\hbar\lambda)\,\rangle = \frac{1 - e^{-\beta\hbar\omega}}{\hbar\,\omega} \int_{-\infty}^{+\infty} \mathrm{d}t\, e^{-i\omega t} \langle A\, B(t)\,\rangle\,. \tag{14}$$

(For details see eqs. 4.13 to 4.14 of ref. [6].)

The time variables of the position operators $\boldsymbol{r}_j(-t - i\hbar\lambda)$ and $\boldsymbol{r}_l \equiv \boldsymbol{r}_l(0)$ may be interchanged by using

$$\langle A(t_1)\, B(t_2)\,\rangle = \langle A(t_1 + \tau)\, B(t_2 + \tau)\,\rangle$$

for two HEISENBERG operators at different times. (The ensemble average is invariant under time translation.) Applying (14) to the integral (13) we obtain

$$\begin{aligned} &\int_{-\infty}^{+\infty} \mathrm{d}t\, e^{-i\omega t} \int_0^\beta \mathrm{d}\lambda\, \langle \sum_{j,l} \exp[-i\,\boldsymbol{q}\cdot\boldsymbol{r}_j]\, \exp[i\,\boldsymbol{q}\cdot\boldsymbol{r}_l(t + i\hbar\lambda)]\,\rangle \\ &\qquad = \frac{1 - e^{-\beta\hbar\omega}}{\hbar\,\omega} \int_{-\infty}^{+\infty} \mathrm{d}t\, e^{-i\omega t}\, \langle \sum_{j,l} \exp[-i\,\boldsymbol{q}\cdot\boldsymbol{r}_j]\, \exp[i\,\boldsymbol{q}\cdot\boldsymbol{r}_l(t)]\,\rangle, \end{aligned}$$

and finally

$$\begin{aligned} q_\alpha\, q_\gamma \operatorname{Re}\sigma_{\alpha\gamma}(\boldsymbol{q},\omega) &= \frac{e^2\,\omega^2}{2} \cdot \frac{1 - e^{-\beta\hbar\omega}}{\hbar\,\omega} \lim_{s\to 0} \int_{-\infty}^{+\infty} \mathrm{d}t\, e^{-(i\omega t + s|t|)}\, \langle \sum_{j,l} \exp[-i\,\boldsymbol{q}\cdot\boldsymbol{r}_j]\, \exp[i\,\boldsymbol{q}\cdot\boldsymbol{r}_l(t)]\,\rangle \\ &= \frac{\pi\, N_0\, e^2\,\omega^2 (1 - e^{-\beta\hbar\omega})}{\hbar\,\omega} \lim_{s\to 0} \frac{1}{2\,\pi} \int_{-\infty}^{+\infty} e^{-i\omega t - s|t|}\, \frac{1}{N_0} \sum_{j,l} \langle \exp[-i\,\boldsymbol{q}\cdot\boldsymbol{r}_j] \exp[i\,\boldsymbol{q}\cdot\boldsymbol{r}_l(t)]\,\rangle. \end{aligned} \tag{15}$$

This formula relates the real part of the conductivity tensor to the FOURIER transform of the "intermediate scattering functions" [7]

$$\frac{1}{N_0}\sum_{j,l}\langle\exp[-i\,\boldsymbol{q}\cdot\boldsymbol{r}_j]\exp[i\,\boldsymbol{q}\cdot\boldsymbol{r}_l(t)]\rangle, \tag{16}$$

as mentioned in the introduction.

An alternate form for (15) is often more convenient for applications. Integrating by parts with respect to time once again, we write instead of (15)

$$q_\alpha q_\gamma \operatorname{Re}\sigma_{\alpha\gamma}(\boldsymbol{q},\omega) = -\frac{e^2}{2}\frac{1-e^{-\beta\hbar\omega}}{\hbar\omega}\lim_{s\to 0}\int_{-\infty}^{+\infty} dt\, e^{-i\omega t-s|t|}\frac{\partial^2}{\partial t^2}\Big\langle\sum_{j,l}\exp[-i\,\boldsymbol{q}\cdot\boldsymbol{r}_j]\exp[i\,\boldsymbol{q}\cdot\boldsymbol{r}_l(t)]\Big\rangle. \tag{17}$$

Both formulae are exact expressions for the real part of the electrical conductivity within the range of validity of the linear response theory of transport.

The Mobility of the Small Polaron

The static conductivity of the small polaron in the HOLSTEIN model was very recently recalculated by SCHNAKENBERG [8] using the GREEN's function technique. (For reference to further work, see ref. [8].) REIK [5] derived an expression for the frequency-dependent mobility $\mu(\omega)$, starting from the KUBO-formula. It is the purpose of this section to deduce his result for the real part of $\mu(\omega)$ from our general formula (17). We follow the notation of REIK's first paper [9], as much as possible, and recall the basic equations for convenience of reference. The total canonically transformed HAMILTONian

$$H = H_0 + H_1$$

is given by the free field parts for the polaron and phonons

$$H_0 = H_{0\,\mathrm{pol}} + H_{0\,\mathrm{ph}} = \tilde{\varepsilon}\sum_p c_p^{+} c_p + \sum_k \hbar\,\omega_k\, a_k^{+} a_k, \tag{18}$$

and an interaction term

$$H_1 = -\frac{J}{2}\sum_p\sum_{\delta=\pm 1} c_p^{+} c_{p+\delta} \cdot\prod_k \exp[-\varrho_k(p,\delta)\{a_k - a_k^{+}\}] \tag{19}$$

which describes the total residual interaction between polaron and lattice. The resonance integral J which occurs in the tight-binding treatment of the one electron in the linear-chain model is considered to be small, so that a perturbation theory of second order in J yields reasonable results. The other quantities contained in the HAMILTONian are defined by

$$\varrho_k(p,\delta) = x_k^{(p+\delta)} - x_k^{(p)};\quad x_k^{(p)} = \alpha_k^{1/2}\sin(k\,p+\pi/4), \tag{20}$$

where p denotes the lattice site in a chain with unit lattice constant, α_k the electron-phonon coupling constant, k the phonon wave vector; $c_p(c_p^{+})$ and $a_k(a_k^{+})$ are fermion and boson-annihilation (creation) operators, respectively. The electron (polaron) position operator r in second quantization is given by

$$r = \sum_p p\, c_p^{+} c_p \tag{21}$$

for all equivalent lattice sites [10].

For the case of one extra electron in the lattice the "intermediate scattering functions" (15) reduce [12] to $\langle e^{-iqr}\, e^{iqr(t)}\rangle$. As in (21) we have omitted the subscript denoting the lattice site, where the

[7] This name is customary in the case of inelastic neutron scattering. There the double sum is broken up into
$(1/N_0)\sum_j\langle e^{-i\,\boldsymbol{q}\cdot\boldsymbol{r}_j} e^{i\boldsymbol{q}\cdot\boldsymbol{r}_j(t)}\rangle + (1/N_0)\sum_{j\neq l}\langle e^{-i\,\boldsymbol{q}\cdot\boldsymbol{r}_j} e^{i\,\boldsymbol{q}\cdot\boldsymbol{r}_l(t)}\rangle$,
the correlation function of a single atom and a pair of atoms, respectively. The dynamical structure factor is defined as the FOURIER transform of the intermediate scattering function.

[8] J. SCHNAKENBERG, Phys. Letters **14**, 266 [1965].

[9] H. G. REIK, Phys. Letters **5**, 236 [1963].

[10] This is exactly valid in a one-band WANNIER representation, where the BLOCH functions are plane waves, so that the WANNIER functions degenerate to δ-functions localized at the lattice points. SEWELL [11] derives the same result by describing the electron wave operator by $\Psi(x) = \sum_p c_p\,\psi_p(x)$, where $\psi_p(x)$ constitute an orthonormal set of localized wave functions of even parity, centred at site p.

[11] G. L. SEWELL, Phys. Rev. **129**, 597 [1963].

[12] In the language of neutron scattering only the incoherent part of the dynamical structure factor given by the correlation function of a single atom is retained.

single electron is localized. The q-dependence of the ensemble average can be separated by expanding the exponentials and taking into account that $n_p = c_p^+ c_p$ is an idempotent operator. The number operator is restricted by the condition

$$\sum_p n_p = 1 \tag{22}$$

if only single-particle states are considered, which is the case in the problem under study. Thus,

$$e^{-iqr} \equiv \exp\{-i\,q \sum_j j\,n_j\} = 1 + \sum_j n_j(e^{-iqj} - 1) = \sum_j e^{-iqj}\, n_j .$$

We now turn to the calculation of the integrand of formula (17). We observe that

$$\frac{\partial^2}{\partial t^2}\langle e^{-iqr}\, e^{iqr(t)}\rangle = -\frac{1}{(i\hbar)^2}\langle [e^{-iqr}, H][e^{iqr(t)}, H]\rangle = \frac{1}{\hbar^2}\sum_{j,l} e^{iq(l-j)}\langle n_j, H][n_l(t), H]\rangle \tag{23}$$

is already of the order J^2, since the number operator n_p commutes with H_0 and the commutator with H_1 is given by

$$[n_j, H] = [n_j, H_1] = \left(-\frac{J}{2}\right)\sum_p \sum_{\delta=\pm 1}\{c_j^+ c_{p+\delta}\,\delta_{jp} - c_p^+ c_j\,\delta_{j,p+\delta}\}\ \prod_k \exp[-\varrho_k(p,\delta)\{a_k - a_k^+\}]. \tag{24}$$

Hence, in a second-order perturbation theory H_1 can be neglected in the exponentials $e^{-\beta H}$ and $e^{\pm itH/\hbar}$. The remaining evaluation of the trace is further simplified by the fact that $e^{itH/\hbar}$ is proportional to the unit operator in our approximation, i. e. $\exp[i\,t\,H/\hbar] = \exp[i\,t\tilde{\varepsilon}/\hbar]\cdot 1$. The time-dependent factors $\exp[\pm i\,t\tilde{\varepsilon}/\hbar]$ cancel, and we are left with

$$\frac{\partial^2}{\partial t^2}\langle e^{-iqr}\, e^{iqr(t)}\rangle = \left(\frac{J}{2\hbar}\right)^2 \sum_{j,l} e^{iq(l-j)} \sum_{p,p'} \sum_{\delta,\delta'=\pm 1} \langle (c_j^+ c_{p+\delta}\,\delta_{jp} - c_p^+ c_j\,\delta_{j,p+\delta})\,(c_l^+ c_{p'+\delta'}\,\delta_{lp'} - c_{p'}^+ c_l\,\delta_{l,p'+\delta'})$$
$$\cdot \prod_k \exp[-\varrho_k(p,\delta)\{a_k - a_k^+\}]\exp[(i\,t/\hbar)\,H_{0\,\mathrm{ph}}]\ \prod_k \exp[-\varrho_k(p',\delta')\{a_k - a_k^+\}]\exp[-(i\,t/\hbar)\,H_{0\,\mathrm{ph}}]\rangle. \tag{25}$$

From (25) it is obvious that the trace over the polaron states and the thermal average of the phonon system can be evaluated independently. Using the theorem

$$e^A\, e^B = e^{A+B}\, e^{1/2[A,B]} \tag{26}$$

which is valid, if the commutator $[A, B]$ commutes with the operators A and B, together with

$$\exp[(i\,t/\hbar)\,H_{0\,\mathrm{ph}}]\ \prod_k \exp[-\varrho_k(p',\delta')\{a_k - a_k^+\}]\exp[-(i\,t/\hbar)\,H_{0\,\mathrm{ph}}] \tag{27}$$
$$= \prod_k \exp[-\varrho_k(p',\delta')\ \{e^{-i\omega_k t}\, a_k - e^{i\omega_k t}\, a_k^+\}],$$

we can write the phonon part of (25) as

$$F_{pp'}^{\delta\delta'} \equiv \langle \prod_k \exp[-\varrho_k(p,\delta)\{a_k - a_k^+\}]\ \exp[-\varrho_k(p',\delta')\ \{e^{-i\omega_k t}\, a_k - e^{i\omega_k t}\, a_k^+\}]\rangle_{\mathrm{ph}}. \tag{28}$$

To simplify this expression, Bloch's theorem can be used.

This theorem states that for any linear combination $Q = \alpha\, a + \gamma\, a^+$ (α, γ c-numbers) of harmonic oscillators displacements, the average over a canonical ensemble with the density operator $\varrho_0 = \exp(-\beta\hbar\omega\, a^+ a)$ is given by the simple relation [13]

$$\langle e^Q\rangle \equiv \frac{\mathrm{Tr}(\exp[-\beta\hbar\omega\, a^+ a]\exp[Q])}{\mathrm{Tr}\exp[-\beta\hbar\omega\, a^+ a]} = \exp[\tfrac{1}{2}\langle Q^2\rangle] = \exp[\tfrac{1}{2}\alpha\gamma\coth\beta\hbar\omega/2]. \tag{29}$$

Applying the theorem to each normal mode k of (28), we obtain

$$F_{pp'}^{\delta\delta'} = \prod_k \exp\left\{-\tfrac{1}{2}[\varrho_k(p,\delta)^2 + \varrho_k(p',\delta')^2]\coth\frac{\beta\hbar\omega_k}{2} - \varrho_k(p,\delta)\,\varrho_k(p',\delta')\,\frac{\cos(t - i\beta\hbar\omega_k/2)}{\sinh\beta\hbar\omega_k/2}\right\}. \tag{30}$$

[13] For a proof, see A. Messiah, Quantum Mechanic, Vol. I, North Holland Publishing Co., Amsterdam, Ch. XII, § 12.

We shall not give the details of the elementary calculation of the ensemble average over the polaron variables. The partition function $Z_{\mathrm{pol}} = \mathrm{Tr}\exp\{-\beta H_{0\,\mathrm{pol}}\}$ is equal to $N\exp[-\beta\tilde{\varepsilon}]$, according to the equivalence of each of the N lattice points. (It cancels against an equal factor in the numerator and will not appear in the final result.) Using (30), we have

$$\frac{\partial^2}{\partial t^2}\langle e^{-iqr}\, e^{iqr(t)}\rangle = \frac{2}{N}\left(\frac{J}{2\hbar}\right)^2 \sum_p \sum_{\delta=\pm 1} (e^{iq\delta}-1)\, F_{pp}^{\delta\delta}\,, \tag{31}$$

or, inserting (20) into (30) and summing over $k = 2\pi\varkappa/N$ (the integer $\varkappa$ lying in the range $-\frac{1}{2}(N-1) \leqq \varkappa \leqq \frac{1}{2}(N-1)$ for a lattice with an odd number N of lattice points),

$$\frac{\partial^2}{\partial t^2}\langle e^{-iqr}\, e^{iqr(t)}\rangle = \frac{4}{N}\left(\frac{J}{2\hbar}\right)^2 (\cos q - 1) \sum_p \exp\left\{-2\,\alpha_k \sin^2\frac{k}{2}\left[\coth\frac{\beta\hbar\omega_k}{2} - \frac{\cos\omega_k(t - i\beta\hbar/2)}{\sinh\beta\hbar\omega_k/2}\right]\right\}. \tag{32}$$

Since the terms of the sum are independent of the lattice sites, the summation over p cancels the $1/N$ factor. Referring back to (17), we write

$$\begin{aligned} q^2\,\mathrm{Re}\,\mu(q,\omega) = {} & \frac{e}{2}\,\frac{1-e^{-\beta\hbar\omega}}{\hbar\omega}\cdot 4\left(\frac{J}{2\hbar}\right)^2 (1-\cos q) \\ & \cdot \lim_{s\to 0}\int_{-\infty}^{\infty+} e^{-i\omega t - s|t|}\exp\left\{-2\,\alpha_k\sin^2\frac{k}{2}\left[\coth\frac{\beta\hbar\omega_k}{2} - \frac{\cos\omega_k(t-i\beta\hbar/2)}{\sinh\beta\hbar\omega_k/2}\right]\right\}, \end{aligned} \tag{33}$$

which can be simplified by introducing the transformation $t' = t - i\beta\hbar/2$.

Finally, the following expression for the real part of the mobility is found:

$$\begin{aligned} \mathrm{Re}\,\mu(q,\omega) = {} & e\beta\left(\frac{J}{2\hbar}\right)^2\left(\frac{\sin(q/2)}{q/2}\right)^2 \frac{\sinh(\beta\hbar\omega/2)}{\beta\hbar\omega/2} \\ & \cdot \lim_{s\to 0}\int_{-\infty}^{+\infty} e^{-i\omega t - s|t|}\exp\left\{-2\,\alpha_k\sin^2\frac{k}{2}\left[\coth\frac{\beta\hbar\omega_k}{2} - \frac{\cos\omega_k t}{\sinh\beta\hbar\omega_k/2}\right]\right\}. \end{aligned} \tag{34}$$

Clearly, in the limit $q\to 0$, this formula reduces to REIK's result as mentioned in the introduction [14]. REIK also gave the expression for the imaginary part of the conductivity and evaluated the integral occuring in (34) by the method of steepest descent. For details, we refer to his paper [5].

It follows immediately from (34) that in HOLSTEIN's linear-chain model of the small polaron, the q-dependence of the real part of the mobility is given by the simple relation

$$\mathrm{Re}\,\mu(q,\omega) = \left(\frac{\sin q/2}{q/2}\right)^2 \mathrm{Re}\,\mu(0,\omega)\,. \tag{35}$$

Acknowledgements

The author wishes to thank his colleague Dr. L. J. WEIGERT for helpful discussions.

[14] Prof. REIK informed the author that both the exponent and the cofactor of the exponential of his result should be multiplied by 2.