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GAUGE TREATMENT OF THE INTRA-COLLISIONAL-FIELD-EFFECT IN ELECTRON TRANSPORT THEORY

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We study the evolution equations of the distribution functions of hot electrons. We show that a convenient choice of the gauge describing the applied uniform electric and magnetic fields considerably simplifies the explicit calculations. The main advantage of our method lies in the possiblility of treating with the same simplicity free electrons (with or without a magnetic field) and Bloch electrons (without a magnetic field). We discuss the influence of the electric field on the collision term of the different transport equations we derive.

1. Introduction

The quantum theory of electrical transport phenomena really originated in 1957 with Kohn and Luttinger's famous paper[1]). Several approximations were there made which limited the theory to (i) linear phenomena with respect to the electric field and (ii) elastic electron–impurities collisions. This formalism was easily applicable to the realistic Bloch electron case. In 1960, P.N. Argyres[2]) extended this type of methods to the case of electrons in the presence of a magnetic field.

From 1960 to 1970, numerous papers were devoted to the study of non-linear phenomena with respect to the electric field[3]); I.B. Levinson[4]) seems to have been the first to recognize the influence of the electric field on the collision term of the transport equation for the electron distribution function (E.D.F.). J.R. Barker[5]) and Barker and Ferry[6]) have investigated since 1973 this effect, which they named the intra-collisional-field-effect (I.C.F.E.); their studies concerned essentially the case of electrons in the absence both of a periodic potential and of a magnetic field.

We propose here a very simple derivation of the intra-collisional-field-effect. Our method is particularly well suited since it can immediately be applied both to the Bloch electrons and to the electrons in the presence of a magnetic field parallel to the electric field. The simplicity of the calculations is

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essentially due to a proper choice of the gauge describing the electric and magnetic fields.

Our paper is organized as follows: in section 2, we briefly recall the basic concepts and the evolution equation of the density matrix. In section 3, we consider the simple case of free electrons submitted to an electric field $\boldsymbol{E}(t)$ and interacting with phonons. This section must in fact be considered as an introduction to the more realistic and interesting Bloch electron case. We choose a gauge in which the electric field $\boldsymbol{E}(t)$ is described by a vector-potential; this choice allows us to diagonalize very simply the Hamiltonian of the electron in the presence of $\boldsymbol{E}(t)$; the corresponding eigenstates are plane waves, quite distinct of the Airy functions obtained in the more usual scalar potential gauge. The evolution equation of the E.D.F. in these quantum states (plane waves) is then obtained and its basic features are discussed. One deduces from there a transport equation for the electron velocity distribution function, which we compare in detail, particularly in what concerns the I.C.F.E., with the evolution equation of the E.D.F. in the plane waves states. In section 4, which constitutes the main part of this work, we turn our attention to the Bloch electron case, for which our formalism can easily be generalized. In the same way than in the free electrons case of section 3, we obtain first the evolution equation of the E.D.F. in the eigenstates of the one-band Hamiltonian of the electron in the presence of the electric field, then the transport equation in the usual Bloch states. Section 5 is devoted to the study of electrons in the presence of a longitudinal magnetic field ($\boldsymbol{E}\parallel\boldsymbol{B}$) for which the I.C.F.E. can easily be investigated with the same methods. A comparison is made with the well-known results of the crossed-fields configuration[7]).

2. Quantum background

Let us consider an independent electron gas, which can interact with an electric field $\boldsymbol{E}(t)$ (possibly time dependent) and a static magnetic field $\boldsymbol{B}$ and which is submitted to the periodic potential $V(\boldsymbol{r})$ of a crystal. These electrons also interact with a phonon gas which we suppose for the sake of simplicity to be in thermal equilibrium. The total electron Hamiltonian thus writes

$$H_{\mathrm{T}}(t) = H(t) + H_{\mathrm{P}} + H_{\mathrm{e\text{-}P}}, \tag{2.1}$$

where $H(t)$ is the electron Hamiltonian in the presence of the applied fields, H_{P} is the phonons Hamiltonian and $H_{\mathrm{e\text{-}P}}$ denotes the electron–phonon interaction Hamiltonian.

I.B. Levinson[4]) showed that, at the lowest order in the electron–phonon coupling, the one-electron density matrix $\mathfrak{f}(t)$ obeys the following equation

$$i\hbar \frac{\partial}{\partial t} \mathfrak{f}(t) - [H(t), \mathfrak{f}(t)] = \mathbf{C}\{\mathfrak{f}(t)\}, \tag{2.2}$$

where the collision term $\mathbf{C}\{\mathfrak{f}(t)\}$ comprises two parts: the first one, $\mathbf{C}_1\{\mathfrak{f}(t)\}$, is due to the emission of phonons

$$\mathbf{C}_1\{\mathfrak{f}(t)\} = -\frac{i}{\hbar} \sum_q |C(q)|^2 (N_q + 1) \int_{-\infty}^{t} dt'\, e^{-i\omega_q(t-t')} \times \left[\chi_q, \exp\left(-\frac{i}{\hbar}\int_{t'}^{t} H(\tau)\, d\tau\right)\chi_q^{+}\mathfrak{f}(t') \exp\left(\frac{i}{\hbar}\int_{t'}^{t} H(\tau)\, d\tau\right)\right] + \text{herm.adj.} \tag{2.3}$$

and the second part, $\mathbf{C}_2\{\mathfrak{f}(t)\}$, is due to the absorption of phonons and can be deduced from the first by the replacements $(N_q + 1) \to N_q$, $\omega_q \to -\omega_q$, $q \to -q$. $C(q)$ characterizes the nature and the strength of the electron–phonon coupling; N_q is the thermal distribution of the phonons of energy $\hbar\omega_q$ and $\chi_q = \exp(iq \cdot r)$.

Eqs. (2.2) and (2.3) can be shown to be equivalent to Barker's eq. (21) in ref. 5, if one neglects the "memory term" and if one retains only the lowest order terms with respect to the electron–phonon coupling strength.

The collision term $\mathbf{C}\{\mathfrak{f}(t)\}$ contains evolution operators such as $\exp(\pm (i/\hbar) \int_{t'}^{t} H(\tau)\, d\tau)$, where $H(t)$, as already stated, is the electron Hamiltonian in the presence of the applied (possibly time-dependent) fields. This dependence of the collision term with the applied fields has been denominated by Barker[5]) the intra-collisional-field-effect (I.C.F.E.).

3. Evolution equation of the distribution function of free electrons in the presence of an electric field

3.1. *Choice of a convenient gauge*

Let us consider at first the most simple case, in which a free electron gas is submitted to a spatially uniform, but possibly time-dependent electric field $E(t)$. The application of such a uniform electric field does not modify the translational invariance of the system. This symmetry property, however, does not appear in the electron Hamiltonian when a scalar potential gauge (gauge $\mathcal{J}$) is used to describe the electric field

$$\text{Gauge } \mathcal{J}\text{: } \phi(r, t) = -eE(t) \cdot r; \quad A(t) = 0 \quad (e < 0), \tag{3.1a}$$

since the electron Hamiltonian in this gauge writes:

$$H_{\mathcal{G}} = \frac{p^2}{2m} - e\boldsymbol{E} \cdot \boldsymbol{r}. \tag{3.1b}$$

If instead the electric field is described by a vector-potential gauge (gauge $\mathcal{G}'$)

$$\text{Gauge } \mathcal{G}'\text{: } \phi(\boldsymbol{r}, t) = 0; \quad \mathbf{A}(t) = -\int_0^t \boldsymbol{E}(\tau)\,\mathrm{d}\tau, \tag{3.2a}$$

the translational invariance property is restored in the electron Hamiltonian itself, which then writes

$$H_{\mathcal{G}}' = \frac{(\boldsymbol{p} - e\mathbf{A}(t))^2}{2m}. \tag{3.2b}$$

We shall now develop some very simple remarks which are basic for the following. The state vectors $|\psi\rangle$ and $|\psi'\rangle$ in the gauges $\mathcal{G}$ and $\mathcal{G}'$ are related by a unitary transformation T. In the $\boldsymbol{r}$-representation, we have

$$\langle \boldsymbol{r} \mid \psi' \rangle = T\langle \boldsymbol{r} \mid \psi \rangle = \exp\Big(\mathrm{i}\frac{e}{\hbar}\boldsymbol{r} \cdot \mathbf{A}(t)\Big)\langle \boldsymbol{r} \mid \psi \rangle. \tag{3.3}$$

As it is well known, the solution of the Schrödinger equation in the gauge $\mathcal{G}$

$$\mathrm{i}\hbar \frac{\mathrm{d}|\psi\rangle}{\mathrm{d}t} = H_{\mathcal{G}}|\psi\rangle \tag{3.4}$$

is (in the $\boldsymbol{r}$-representation)

$$\langle \boldsymbol{r} \mid \psi(t) \rangle = \Omega^{-1/2} \exp\Big(\mathrm{i}\boldsymbol{k}(t) \cdot \boldsymbol{r} - \frac{\mathrm{i}}{\hbar}\int_0^t \frac{\hbar^2 \boldsymbol{k}(\tau)^2}{2m}\,\mathrm{d}\tau\Big) \tag{3.5}$$

(Ω is the volume of the sample) with

$$\boldsymbol{k}(t) = \boldsymbol{k}(0) - \frac{e}{\hbar}\mathbf{A}(t). \tag{3.6}$$

This implies that the state vector in the gauge $\mathcal{G}'$ is (in the $\boldsymbol{r}$-representation)

$$\langle \boldsymbol{r} \mid \psi' \rangle = \Omega^{-1/2} \exp\Big(\mathrm{i}\boldsymbol{k}(0) \cdot \boldsymbol{r} - \frac{\mathrm{i}}{\hbar}\int_0^t \frac{\hbar^2 \boldsymbol{k}(\tau)^2}{2m}\,\mathrm{d}\tau\Big) \tag{3.7}$$

and therefore the Schrödinger equation in the gauge $\mathcal{G}'$

$$\mathrm{i}\hbar \frac{\mathrm{d}|\psi'\rangle}{\mathrm{d}t} = H_{\mathcal{G}'}|\psi'\rangle \tag{3.8}$$

gives rise to the eigenvalue equation

$$H_{\mathscr{J}'}|\psi'\rangle = \frac{\hbar^2(k(0)-(e/\hbar)A(t))^2}{2m}|\psi'\rangle. \tag{3.9}$$

In the following we shall denote the eigenstates of $H_{\mathscr{J}'}$ by $|K\rangle$ and the associated eigenvalues by $\epsilon(K-(e/\hbar)A(t))$. The state vector deduced from $|K\rangle$ by the unitary transformation $T^\dagger$ will from now on be denoted by $|k\rangle$. These states possess the following property: they are eigenstates of the free electron Hamiltonian H_0 (without the electric field) with the eigenvalues $\epsilon(k(t))$.

It is then straightforward to deduce from eq. (2.2) the equation for the electron distribution function (E.D.F.) in the $|K\rangle$-states, defined by

$$f(K,t) = \langle K|\mathfrak{f}(t)|K\rangle. \tag{3.10}$$

Since the medium we consider is homogeneous, the electron density matrix must be translationally invariant; it commutes then with the impulsion operator p and with $H(t)$, so that the left-hand side (l.h.s.) of the equation for the E.D.F. reduces to $\partial f(K,t)/\partial t$.

It's however in the calculation of the collision term (2.3) that the vector-potential gauge choice proves to be the most efficient. Let us calculate in the $\{|K\rangle\}$ basis the diagonal matrix element of one of the terms of the commutators involved in expression (2.3), for instance

$$A_K = \langle K|\chi_q \exp\left[-\frac{i}{\hbar}\int_{t'}^{t} H(\tau)\,d\tau\right]\chi_q^\dagger\,\mathfrak{f}(t')\exp\left[\frac{i}{\hbar}\int_{t'}^{t} H(\tau)\,d\tau\right]|K\rangle. \tag{3.11}$$

Since

$$\langle K|\chi_q|K'\rangle = \delta_{K,K'+q} \tag{3.12}$$

one obtains straightforwardly

$$A_K = \sum_{K'} |\langle K|\chi_q|K'\rangle|^2 \exp\left\{-\frac{i}{\hbar}\int_{t'}^{t}\left(\epsilon\left(K'-\frac{e}{\hbar}A(\tau)\right)\right.\right.$$
$$\left.\left. -\,\epsilon\left(K-\frac{e}{\hbar}A(\tau)\right)\right)d\tau\right\} f(K,t') \tag{3.13}$$

Each matrix element of the collision term can be expressed in a similar way, which yields the following equation for the E.D.F. over the $|K\rangle$-states

$$\frac{\partial}{\partial t} f(K,t) = \int_{-\infty}^{t} dt' \sum_{K'} \{P(K',K;t,t')f(K',t') - P(K,K';t,t')f(K,t')\} \tag{3.14a}$$

with

$$P(\boldsymbol{K}, \boldsymbol{K}'; t, t') = \frac{2}{\hbar^2} \operatorname{Re} \sum_{q} \sum_{\eta=-1,+1} |\langle \boldsymbol{K}|\chi_{\eta q}|\boldsymbol{K}'\rangle|^2 |C(\boldsymbol{q})|^2 \Big(N_q + \frac{1}{2} + \frac{\eta}{2}\Big)$$

$$\times \exp\Big\{-\frac{\mathrm{i}}{\hbar}\int_{t'}^{t} \mathrm{d}\tau \Big(\epsilon\Big(\boldsymbol{K}' - \frac{e}{\hbar}\mathbf{A}(\tau)\Big) - \epsilon\Big(\boldsymbol{K} - \frac{e}{\hbar}\mathbf{A}(\tau)\Big) + \eta\hbar\omega_q\Big)\Big\}. \tag{3.14b}$$

$\eta = +1$ (or -1) corresponds to the phonon emission (or absorption) processes.

Let us now comment about the evolution equation (3.14). Several remarks can be made:

(i) There is no drift term in the l.h.s. and the whole effect of the electric field is included in the collision term (r.h.s.);

(ii) The collision term is non-Markoffian, since it involves retarded distribution functions;

(iii) Even in the case of a *static* electric field, one cannot rewrite the collision term under the form of a convolution product since the probabilities $P(\boldsymbol{K}, \boldsymbol{K}'; t, t')$ are not functions of the time difference $(t - t')$; this implies that one cannot find by the usual technics a Markoffian equation for $f(\boldsymbol{K}, t)$ in the asymptotic limit $(t \to \infty)$;

(iv) The stationary state in a static electric field $\boldsymbol{E}(t) = \boldsymbol{E}_0$ does not correspond to the condition that one could expect $\partial f(\boldsymbol{K}, t)/\partial t = 0$.

In order to clarify this last statement, let us calculate the electric current density

$$\boldsymbol{J} = \frac{e}{\Omega} \operatorname{Tr} \hat{\boldsymbol{v}} \mathbf{f}(t), \tag{3.15}$$

where $\hat{\boldsymbol{v}}$ is the electron velocity operator

$$\hat{\boldsymbol{v}} = \frac{\boldsymbol{p} - e\boldsymbol{A}(t)}{m}. \tag{3.16}$$

In the case of a static field, one gets

$$\boldsymbol{J} = \frac{e}{\Omega} \sum_{\boldsymbol{K}} \frac{\hbar\mathbf{K} + e\mathbf{E}_0 t}{m} f(\mathbf{K}, t) = \frac{e}{\Omega} \sum_{\boldsymbol{K}} \frac{\hbar\mathbf{K}}{m} f(\mathbf{K}, t) + \frac{ne^2\mathbf{E}_0 t}{m} \tag{3.17}$$

(n is the electron density). In a steady-state regime, $f(\boldsymbol{K}, t)$ cannot be time independent, (i.e. $\partial f(\boldsymbol{K}, t)/\partial t \neq 0$), since the gauge current $(ne^2\mathbf{E}_0 t/m)$ must be counterbalanced by a term linear in t. This remark will be clarified in the next paragraph, in which we shall determine the velocity distribution $\phi(\boldsymbol{v}, t)$.

3.2. *Velocity distribution in a uniform electric field*

The expectation value of the electron velocity in a state $|\boldsymbol{K}\rangle$ is simply

$$\boldsymbol{v} = \langle \boldsymbol{K}|\hat{\boldsymbol{v}}|\boldsymbol{K}\rangle = \frac{\hbar \boldsymbol{K} - e\boldsymbol{A}(t)}{m} \left(= \frac{\hbar \boldsymbol{k}}{m}\right). \tag{3.1}$$

This relation can be inverted, which defines $\boldsymbol{K}$ as a function of $\boldsymbol{v}$ and t,

$$\boldsymbol{K}(\boldsymbol{v}, t) = \frac{m\boldsymbol{v} + e\boldsymbol{A}(t)}{\hbar}. \tag{3.1}$$

The velocity distribution $\phi(\boldsymbol{v}, t)$ is then obtained by substituting in $f(\boldsymbol{K}, t)$ t
$\boldsymbol{K}$-vector by its expression (3.19) as a function of $\boldsymbol{v}$

$$\phi(\boldsymbol{v}, t) = f(\boldsymbol{K}(\boldsymbol{v}, t), t). \tag{3.2}$$

One verifies easily that

$$\frac{\partial}{\partial t} f(\boldsymbol{K}, t) = \frac{\partial}{\partial t}\phi(\boldsymbol{v}, t) + \frac{e\boldsymbol{E}}{m} \cdot \nabla_v \phi(\boldsymbol{v}, t) \tag{3.2}$$

and that

$$f(\boldsymbol{K}, t') = \phi\left(\boldsymbol{v} + \frac{e}{m}(\boldsymbol{A}(t) - \boldsymbol{A}(t')), t'\right). \tag{3.2}$$

In the same way, the energy variation in the transition $\boldsymbol{K} \to \boldsymbol{K}'$ can expressed as a function of the velocities $\boldsymbol{v}$ and $\boldsymbol{v}'$

$$\epsilon\left(\boldsymbol{K}' - \frac{e}{\hbar}\boldsymbol{A}(\tau)\right) - \epsilon\left(\boldsymbol{K} - \frac{e}{\hbar}\boldsymbol{A}(\tau)\right) = \frac{1}{2} m(v'^2 - v^2) + e(\boldsymbol{v}' - \boldsymbol{v}) \cdot (\boldsymbol{A}(t) - \boldsymbol{A}(\tau)). \tag{3.2}$$

One thus obtains for the electron velocity distribution the transport equ tion

$$\frac{\partial}{\partial t}\phi(\boldsymbol{v}, t) + \frac{e\boldsymbol{E}}{m} \cdot \nabla_v \phi(\boldsymbol{v}, t) = \int_{-\infty}^{t} \mathrm{d}t' \sum_{v'} \left\{ \Pi(\boldsymbol{v}', \boldsymbol{v}; t, t')\phi\left(\boldsymbol{v}' + \frac{e}{m}(\boldsymbol{A}(t) - \boldsymbol{A}(t')), \right.\right.$$
$$\left.\left. - \Pi(\boldsymbol{v}, \boldsymbol{v}'; t, t')\phi\left(\boldsymbol{v} + \frac{e}{m}(\boldsymbol{A}(t) - \boldsymbol{A}(t')), t'\right)\right\}, \tag{3.24}$$

with

$$\Pi(\boldsymbol{v}, \boldsymbol{v}'; t, t') = \frac{2}{\hbar^2} \mathrm{Re} \sum_{q} \sum_{\eta = -1, +1} \delta_{\boldsymbol{v}, \boldsymbol{v}' + (\eta\hbar \boldsymbol{q}/m)} |C(\boldsymbol{q})|^2 \left(N_q + \frac{1}{2} + \frac{\eta}{2}\right)$$
$$\times \exp\left\{-\frac{\mathrm{i}}{\hbar}\int_{t'}^{t} \mathrm{d}\tau \left(\frac{m}{2}(v'^2 - v^2) + e(\boldsymbol{v}' - \boldsymbol{v}) \cdot (\boldsymbol{A}(t) - \boldsymbol{A}(\tau)) + \eta\hbar\omega_q\right)\right\}. \tag{3.24}$$

This result can be understood as follows: as we stated previously, states $|\boldsymbol{K}\rangle$ and $|\boldsymbol{k}\rangle$ are related by a unitary transformation T (see eq. (3.3)) which corresponds to the change of gauge $\mathcal{J} \to \mathcal{J}'$. Therefore the operator $T^{\dagger}\mathfrak{f}(t)T$ represents the density matrix $\tilde{\mathfrak{f}}(t)$ when the scalar potential gauge $\mathcal{J}$ is used. Thus

$$\langle \boldsymbol{K}|\mathfrak{f}(t)|\boldsymbol{K}\rangle = \langle \boldsymbol{k}|T^{\dagger}\mathfrak{f}(t)T|\boldsymbol{k}\rangle = \langle \boldsymbol{k}|\tilde{\mathfrak{f}}(t)|\boldsymbol{k}\rangle, \tag{3.25}$$

so that

$$\phi(\boldsymbol{k}, t) = \langle \boldsymbol{k}|\tilde{\mathfrak{f}}(t)|\boldsymbol{k}\rangle. \tag{3.26}$$

$\phi(\boldsymbol{k}, t)$ is the electron distribution function in the $|\boldsymbol{k}\rangle$-states, which, as already stated, are the eigenstates of the free electron Hamiltonian H_0, and so, apart from a constant numerical factor, it is the velocity distribution function.

The transport equation (3.24) for the electron velocity distribution function is identical to Barker's result[5]); it deserves nevertheless some commentaries:

(i) We recover the usual drift term in the l.h.s. and the transition probabilities in the collision term do depend on the electric field: this dependence constitutes the intra-collisional-field-effect (I.C.F.E.);

(ii) The collision term is non-Markoffian; moreover it involves distribution functions which depend on the modified velocities

$$v^{*(\prime)} = \boldsymbol{v}^{(\prime)} + \frac{e}{m}(\mathbf{A}(t) - \mathbf{A}(t')). \tag{3.27}$$

The usual velocity dependence can only be restored by a coarse-graining of the distribution function in the velocity space, i.e. by the approximation

$$\phi\left(\boldsymbol{v} + \frac{e}{m}(\mathbf{A}(t) - \mathbf{A}(t')), t'\right) \approx \phi(\boldsymbol{v}, t'). \tag{3.28}$$

(iii) In the case of a static electric field, the collision term can be recast into a Markoffian form in the asymptotic limit ($t \to \infty$) by the usual technics[5]);

(iv) The velocity distribution $\phi(\boldsymbol{v}, t)$ can be used to calculate the electric current density as

$$\boldsymbol{J} = \frac{e}{\Omega}\int \mathrm{d}^3\boldsymbol{v}\, \boldsymbol{v}\phi(\boldsymbol{v}, t) \tag{3.29}$$

and, as expected, for a static electric field $\boldsymbol{E}_0$, $\phi(\boldsymbol{v}, t)$ is time independent in a steady-state regime. This proves in turn that, in this stationary case, the electron distribution function in $|\boldsymbol{K}\rangle$-states, $f(\boldsymbol{K}, t)$, is time dependent, as it was noticed after eq. (3.17), since then

$$f(\boldsymbol{K}, t) = \phi(\boldsymbol{v}) \tag{3.30}$$

is only a function of $\boldsymbol{K} + e\boldsymbol{E}_0 t/\hbar$.

4. Bloch electrons case (zero magnetic field)

We shall now treat the more realistic case of Bloch electrons submitted to a spatially uniform, but possibly time-dependent electric field. We shall assume for the sake of simplicity that we neglect interband transitions; thus the electrons always remain in the same band ν.

4.1. *Gauge choice and basis states*

The importance of the preceding section does not lie in the final results, part of them having already been established by another way, but in the use of a convenient gauge for the electric field. Similarly, the vector-potential gauge will prove to be equally well suited to the derivation of a transport equation for the E.D.F. of Bloch electrons.

We need to deal with the properties of three different Hamiltonians:

$$H_0 = \frac{p^2}{2m} + V(\boldsymbol{r}), \tag{4.1a}$$

$$H_{\mathcal{G}} = \frac{p^2}{2m} + V(\boldsymbol{r}) - e\boldsymbol{E}(t)\cdot\boldsymbol{r}, \tag{4.1b}$$

$$H_{\mathcal{G}'} = \frac{(\boldsymbol{p} - e\boldsymbol{A}(t))^2}{2m} + V(\boldsymbol{r}). \tag{4.1c}$$

H_0 describes simply a Bloch electron in the periodic lattice potential $V(\boldsymbol{r})$; $H_{\mathcal{G}}$ and $H_{\mathcal{G}'}$ correspond both to the same Bloch electron submitted in addition to the uniform electric field $\boldsymbol{E}(t)$; $H_{\mathcal{G}}$ is written with the scalar potential gauge $\mathcal{G}$ whereas we have used the vector-potential gauge $\mathcal{G}'$ for $H_{\mathcal{G}'}$.

Let us recall two properties satisfied by the different Hamiltonians:

(i) The state vectors $|\psi\rangle$ and $|\psi'\rangle$ in the gauges $\mathcal{G}$ and $\mathcal{G}'$ obey the two Schrödinger equations (3.4) and (3.8) and they are related by a unitary transformation T defined by eq. (3.3);

(ii) This same unitary operator T transforms H_0 into $H_{\mathcal{G}'}$. Effectively, one easily verifies that

$$H_{\mathcal{G}'} = TH_0T^{\dagger}. \tag{4.2}$$

Accordingly, let us label $|\boldsymbol{k}\rangle$ and $\epsilon(\boldsymbol{k})$ the eigenstates and the eigenvalues of H_0 (we omit the band index ν for the moment). We know that

$$\langle \boldsymbol{r} \mid \boldsymbol{k}\rangle = \Omega^{-1/2}\exp(\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r})u_{\boldsymbol{k}}(\boldsymbol{r}) \tag{4.3}$$

are the usual Bloch functions. If we denote by $|\boldsymbol{K}\rangle$ and $E(\boldsymbol{K})$ the eigenstates and the eigenvalues of $H_{\mathcal{G}'}$, we derive immediately from eqs. (3.3) and (4.2) relations between the eigenstates $|\boldsymbol{K}\rangle$ and $|\boldsymbol{k}\rangle$ on the one hand, and between the eigenvalues $E(\boldsymbol{K})$ and $\epsilon(\boldsymbol{k})$ on the other hand:

$$|\boldsymbol{K}\rangle = T|\boldsymbol{k}\rangle \quad (4.4a); \quad E(\boldsymbol{K}) = \epsilon(\boldsymbol{k}). \tag{4.4b}$$

Then we arrive to the following expression for the eigenstates of $H_{\mathcal{J}'}$, deduced from eqs. (4.3) and (4.4a):

$$\langle \boldsymbol{r} \mid \boldsymbol{K}\rangle = \Omega^{-1/2}\exp(\mathrm{i}\boldsymbol{K}\cdot\boldsymbol{r})w_{\boldsymbol{K}}(\boldsymbol{r}), \tag{4.5}$$

with

$$\boldsymbol{K} = \boldsymbol{k} + \frac{e}{\hbar}\mathbf{A}(t) \tag{4.6}$$

and

$$w_{\boldsymbol{K}}(\boldsymbol{r}) = u_{\boldsymbol{K}-(e/\hbar)\mathbf{A}(t)}(\boldsymbol{r}). \tag{4.7}$$

So we proved that the eigenfunctions of $H_{\mathcal{J}'}$ are also Bloch functions; this is quite evident on the expression of $H_{\mathcal{J}'}$, which possesses exactly the same translational invariance property as H_0.

Here we can introduce, as in the preceding section on free electrons, the vector $\boldsymbol{k}(t)$, defined by eq. (3.6), with $\boldsymbol{k}(0) = \boldsymbol{K}$. Expressed in terms of $\boldsymbol{k}(t)$, the results useful for the following are finally (we insert the band index ν omitted until now):

$$H_{\mathcal{J}'}|\nu\boldsymbol{K}\rangle = \epsilon_\nu(\boldsymbol{k}(t))|\nu\boldsymbol{K}\rangle \tag{4.8}$$

and

$$\langle \boldsymbol{r} \mid \nu\boldsymbol{K}\rangle = T\Omega^{-1/2}\exp(\mathrm{i}\boldsymbol{k}(t)\cdot\boldsymbol{r})u_{\nu\boldsymbol{k}(t)}(\boldsymbol{r}). \tag{4.9}$$

It is at present straightforward to deduce from eq. (2.2) the equation of evolution of the E.D.F. in the eigenstates $|\nu\boldsymbol{K}\rangle$ of $H_{\mathcal{J}'}$, defined by

$$f_\nu(\boldsymbol{K}, t) = \langle \nu\boldsymbol{K}|\mathfrak{f}(t)|\nu\boldsymbol{K}\rangle. \tag{4.10}$$

For the l.h.s., we simply get $\partial f_\nu(\boldsymbol{K}, t)/\partial t$. In the r.h.s. collision term, we have to evaluate expressions such as

$$B_\nu(\boldsymbol{K}) = \langle \nu\boldsymbol{K}|\chi_{\boldsymbol{q}}\exp\left[-\frac{\mathrm{i}}{\hbar}\int_{t'}^{t} H(\tau)\,d\tau\right]\chi_{\boldsymbol{q}}^{\dagger}\mathfrak{f}(t')\exp\left[\frac{\mathrm{i}}{\hbar}\int_{t'}^{t} H(\tau)\,\mathrm{d}\tau\right]|\nu\boldsymbol{K}\rangle. \tag{4.11}$$

Since we assumed that the electrons always remain within the same energy band ν, we immediately get

$$B_\nu(\boldsymbol{K}) = \sum_{\boldsymbol{K}'}\sum_{\boldsymbol{K}''}\langle \nu\boldsymbol{K}|\chi_{\boldsymbol{q}}|\nu\boldsymbol{K}'\rangle\langle \nu\boldsymbol{K}'|\chi_{\boldsymbol{q}}^{\dagger}|\nu\boldsymbol{K}''\rangle$$

$$\times\exp\left\{-\frac{i}{\hbar}\int_{t'}^{t}(\epsilon_\nu(\boldsymbol{k}'(\tau)) - \epsilon_\nu(\boldsymbol{k}(\tau)))\,\mathrm{d}\tau\right\}f_\nu(\boldsymbol{K}'', t'). \tag{4.12}$$

In the appendix, we show that the product $\langle \nu \boldsymbol{K}|\chi_{\boldsymbol{q}}|\nu \boldsymbol{K}'\rangle\langle \nu \boldsymbol{K}'|\chi^{\dagger}_{\boldsymbol{q}}|\nu \boldsymbol{K}''\rangle$ differs from zero only if $\boldsymbol{K}'' = \boldsymbol{K}$ and takes the value

$$\delta_{\boldsymbol{K},\boldsymbol{K}''}|\langle \nu \boldsymbol{K}|\chi_{\boldsymbol{q}}|\nu \boldsymbol{K}'\rangle|^2 = \delta_{\boldsymbol{K},\boldsymbol{K}''} \sum_{\boldsymbol{g}} \delta_{\boldsymbol{K}'-\boldsymbol{K}+\boldsymbol{q},\boldsymbol{g}} \left| \frac{1}{c} \int_{c} \mathrm{d}\boldsymbol{r} w^{*}_{\nu \boldsymbol{K}}(\boldsymbol{r}) w_{\nu,\boldsymbol{K}-\boldsymbol{q}}(\boldsymbol{r}) \right|^2, \tag{4.13}$$

where $\boldsymbol{g}$ is a reciprocal lattice vector and c is the volume of an elementary cell of the crystal. The expression of $B_\nu(\boldsymbol{K})$ is quite similar to the corresponding term $A(\boldsymbol{K})$ calculated in section 3. Each term of the r.h.s. of eq. (2.2) can be calculated in a similar fashion. Finally the evolution equation of $f_\nu(\boldsymbol{K}, t)$ looks identical to eq. (3.14); the only differences lie in the meaning of $|\nu \boldsymbol{K}\rangle$ and $\epsilon_\nu(\boldsymbol{k}(t))$ which here are the eigenstates and eigenvalues of the Bloch electrons in the presence of the electric field described by a vector-potential gauge.

All the comments we made about (3.14) are still appropriate; nevertheless, the contribution of the electrons in band ν to the electric current has now the expression

$$\boldsymbol{J}_\nu = \frac{e}{\Omega} \sum_{\boldsymbol{K}} \frac{1}{\hbar} \nabla_{\boldsymbol{K}} \epsilon_\nu \left(\boldsymbol{K} - \frac{e}{\hbar} \mathbf{A}(t) \right) f_\nu(\boldsymbol{K}, t). \tag{4.14}$$

4.2. *Transport equation in the usual Bloch states*

We have just derived the evolution equation for the E.D.F. in the $|\nu \boldsymbol{K}\rangle$ eigenstates of the Hamiltonian $H_{\mathcal{J}'}$. We want now to deduce the transport equation for the E.D.F. in the usual Bloch states, which are the eigenstates of the Hamiltonian H_0 in the absence of the electric field. This is quite easy; starting from eqs. (4.10) and (4.4a), we obtain

$$f_\nu(\boldsymbol{K}, t) = \langle \nu \boldsymbol{K}|\mathfrak{f}(t)|\nu \boldsymbol{K}\rangle = \langle \nu \boldsymbol{k}|T^{\dagger}\mathfrak{f}(t)T|\nu \boldsymbol{k}\rangle. \tag{4.15}$$

Since $\mathfrak{f}(t)$ and $T^{\dagger}\mathfrak{f}(t)T$ represent exactly the same physical properties expressed in the two different gauges $\mathcal{J}'$ and $\mathcal{J}$, the matrix element $\langle \nu \boldsymbol{k}|T^{\dagger}\mathfrak{f}(t)T|\nu \boldsymbol{k}\rangle$, which we shall label $\phi_\nu(\boldsymbol{k}, t)$, is the E.D.F. in the usual Bloch states $|\nu \boldsymbol{k}\rangle$.

The steps of the derivation of the transport equation for $\phi_\nu(\boldsymbol{k}, t)$ are quite analogous to those described by eqs. (3.21) to (3.23) for the free electrons case, and we obtain

$$\frac{\partial}{\partial t} \phi_\nu(\boldsymbol{k}, t) + \frac{e\boldsymbol{E}}{\hbar} \cdot \nabla_{\boldsymbol{k}} \phi_\nu(\boldsymbol{k}, t) = \int_{-\infty}^{t} \mathrm{d}t' \sum_{\boldsymbol{k}'} \{ \Pi_\nu(\boldsymbol{k}', \boldsymbol{k}; t, t')$$
$$\times \phi_\nu\left(\boldsymbol{k}' + \frac{e}{\hbar}(\mathbf{A}(t) - \mathbf{A}(t')), t'\right) - \Pi_\nu(\boldsymbol{k}, \boldsymbol{k}'; t, t') \phi_\nu\left(\boldsymbol{k} + \frac{e}{\hbar}(\mathbf{A}(t) - \mathbf{A}(t')), t'\right) \Big\}, \tag{4.16a}$$

with

$$\Pi_\nu(\boldsymbol{k}, \boldsymbol{k}'; t, t') = \frac{2}{\hbar^2} \operatorname{Re} \sum_{\boldsymbol{q}} \sum_{\eta=-1,+1} |\langle \nu \boldsymbol{k} | \chi_{\eta \boldsymbol{q}} | \nu \boldsymbol{k}' \rangle|^2 |C(\boldsymbol{q})|^2 \left(N_{\boldsymbol{q}} + \frac{1}{2} + \frac{\eta}{2} \right)$$
$$\times \exp\left\{ -\frac{i}{\hbar} \int_{t'}^{t} d\tau \left(\epsilon_\nu \left(\boldsymbol{k}' + \frac{e}{\hbar} (\mathbf{A}(t) - \mathbf{A}(\tau)) \right) \right.\right.$$
$$\left.\left. - \epsilon_\nu \left(\boldsymbol{k} + \frac{e}{\hbar} (\mathbf{A}(t) - \mathbf{A}(\tau)) \right) + \eta \hbar \omega_{\boldsymbol{q}} \right) \right\}. \tag{4.16b}$$

This transport equation is valid at the lowest order in the electron–phonon coupling, whatever the details of the band structure. Exactly as in the free electrons case, the l.h.s. of the transport equation contains a drift term, and the transition probabilities $\Pi_\nu(\boldsymbol{k}, \boldsymbol{k}'; t, t')$ depend explicitly on the electric field through the vector-potential. This dependence constitutes the intra-collisional-field-effect in the Bloch electrons case. All the comments on the non-Markoffian character of the collision term for the free electrons velocity distribution function $\phi(\boldsymbol{v}, t)$ can be repeated again for $\phi_\nu(\boldsymbol{k}, t)$. The contribution of the electrons in band ν to the electric current density is given by

$$\boldsymbol{J}_\nu = \frac{e}{\Omega} \sum_{\boldsymbol{k}} \frac{1}{\hbar} \nabla_{\boldsymbol{k}} \epsilon_\nu(\boldsymbol{k}) \phi_\nu(\boldsymbol{k}, t). \tag{4.17}$$

From eq. (4.17) and from the definition of $\phi_\nu(\boldsymbol{k}, t)$, we verify easily that, for a static electric field $\boldsymbol{E}_0$, the stationary distribution function $f_\nu(\boldsymbol{K}, t)$ remains time dependent since it is only a function of $\boldsymbol{K} + (e\boldsymbol{E}_0 t/\hbar)$.

5. Free electrons in the presence of uniform electric and magnetic fields

5.1. *Parallel fields case*

The strong analogy which exists between this problem and the problem treated in section 3 allows us to be rather succinct in the derivations. The most convenient gauge to describe the two uniform fields $\boldsymbol{E}$ and $\boldsymbol{B}$ assumed to be parallel to the z-axis is

$$\text{Gauge } \mathcal{G}_B':\ \phi(\boldsymbol{r}, t) = 0; \quad \mathbf{A} = \left(A_x = 0,\ A_y = Bx,\ A_z = -\int_0^t E(\tau)\, d\tau \right). \tag{5.1}$$

The magnetic field $\boldsymbol{B}$ is always static; on the contrary the electric field $\boldsymbol{E}(t)$ can vary with time. The electron Hamiltonian is in this gauge

$$H_{\mathcal{G}_B'} = \frac{1}{2m} [p_x^2 + (p_y - eBx)^2 + (p_z - eA_z(t))^2]. \tag{5.2}$$

It can easily be checked that, exactly as plane waves were eigenstates of the Hamiltonian (3.2b), the Landau states

$$\psi'_\Lambda(r) = \langle r \mid \Lambda\rangle = \Omega^{-1/2} \exp i(K_y y + K_z z)\phi_n\left(x + \frac{\hbar K_y}{m\omega_c}\right) \tag{5.3}$$

are eigenstates of the Hamiltonian $H_{\mathcal{J}'_B}$. Λ is an index which summarizes the three usual quantum numbers n, K_y and K_z; $\omega_c = |e|B/m$. We have

$$H_{\mathcal{J}'_B}|\Lambda\rangle = \epsilon_\Lambda(t)|\Lambda\rangle, \tag{5.4a}$$

where

$$\epsilon_\Lambda(t) = \epsilon_n\left(K_z - \frac{e}{\hbar}A_z(t)\right) = \left(n + \frac{1}{2}\right)\hbar\omega_c + \frac{(\hbar K_z - eA_z(t))^2}{2m}. \tag{5.4b}$$

The E.D.F. in the eigenstates $|\Lambda\rangle$ of $H_{\mathcal{J}'_B}$ is defined by

$$f_n(K_y, K_z, t) = \langle\Lambda|\mathfrak{f}(t)|\Lambda\rangle. \tag{5.5}$$

In the presence of a magnetic field, there is no gauge in which the electron Hamiltonian is translationally invariant. But, if the fields $\boldsymbol{E}$ and $\boldsymbol{B}$ are uniform, the physical properties of the electron gas must also be uniform; therefore the E.D.F. $f_n(K_y, K_z, t)$ should not depend on K_y, since the quantity $\hbar K_y/m$ represents the mean abscissa of an electron in the state $|\Lambda\rangle$; so we shall simply write the E.D.F. as $f_n(K_z, t)$.

As before, an evolution equation for the E.D.F. can be derived from eq. (2.2). In the calculation of the diagonal matrix elements of the collision operator we encounter expressions such as

$$C_\Lambda = \langle\Lambda|\chi_q \exp\left[-\frac{i}{\hbar}\int_{t'}^{t} H(\tau)\,d\tau\right]\chi_q^\dagger\mathfrak{f}(t')\exp\left[\frac{i}{\hbar}\int_{t'}^{t} H(\tau)\,d\tau\right]|\Lambda\rangle, \tag{5.11a}$$

or

$$C_\Lambda = \sum_{\Lambda'}\sum_{\Lambda''}\langle\Lambda|\chi_q|\Lambda'\rangle\langle\Lambda'|\chi_q^\dagger|\Lambda''\rangle\langle\Lambda''|\mathfrak{f}(t')|\Lambda\rangle$$
$$\times \exp\left\{-\frac{i}{\hbar}\int_{t'}^{t} d\tau\left(\epsilon_{n'}\left(K'_z - \frac{e}{\hbar}A_z(\tau)\right) - \epsilon_n\left(K_z - \frac{e}{\hbar}A_z(\tau)\right)\right)\right\}. \tag{5.11b}$$

P.N. Argyres[2]) has proved that, owing to the summation over $\boldsymbol{q}$ in C_Λ, the only terms different from zero in C_Λ correspond to $\Lambda'' = \Lambda$. We find finally that the E.D.F. $f_n(K_z, t)$ obeys the equation

$$\frac{\partial}{\partial t}f_n(K_z, t) = \int_{-\infty}^{t} dt' \sum_{n'K'_z}\{W_{n'n}(K'_z, K_z; t, t')f_{n'}(K'_z, t')$$
$$- W_{nn'}(K_z, K'_z; t, t')f_n(K_z, t)\} \tag{5.12a}$$

with

$$W_{nn'}(K_z, K'_z; t, t') = \frac{2}{\hbar^2} \mathrm{Re} \sum_{q} \sum_{\eta=-1,+1} \delta_{K_z, K'_z+\eta q_z} |J_{nn'}(q_x, q_y)|^2 |C(q)|^2 \left(N_q + \frac{1}{2} + \frac{\eta}{2}\right)$$

$$\times \exp\left\{-\frac{i}{\hbar} \int_{t'}^{t} d\tau \left(\epsilon_{n'}\left(K'_z - \frac{e}{\hbar} A_z(\tau)\right)\right.\right.$$

$$\left.\left. - \epsilon_n\left(K_z - \frac{e}{\hbar} A_z(\tau)\right) + \eta\hbar\omega_q\right)\right\} \tag{5.12b}$$

and where

$$|J_{nn'}(q_x, q_y)|^2 = \left| \int_{-\infty}^{+\infty} \phi_n^*(x) \exp(iq_x x) \phi_{n'}\left(x + \frac{hq_y}{m\omega_c}\right) dx \right|^2 .$$

Again we can repeat all the comments following eq. (3.14), except for the electric current density, which now expresses as

$$J_z = \frac{e}{\Omega} \sum_{nK_yK_z} \frac{\hbar K_z - eA_z(t)}{m} f_n(K_z, t). \tag{5.13}$$

We can transform the equation satisfied by $f_n(K_z, t)$ in order to get a transport equation for the velocity distribution function of the electrons. Since the expectation value in a state $|\Lambda\rangle$ of the electron velocity (directed along the fields) is

$$v_z = \frac{\hbar K_z - eA_z(t)}{m}, \tag{5.14}$$

the velocity distribution function is defined by

$$\phi_n(v_z, t) = f_n(K_z(v_z, t), t) \tag{5.15}$$

and it obeys the transport equation

$$\frac{\partial}{\partial t} \phi_n(v_z, t) + \frac{eE}{m} \frac{\partial}{\partial v_z} \phi_n(v_z, t) = \int_{-\infty}^{t} dt' \sum_{n'K'_z} \left\{\Omega_{n'n}(v'_z, v_z; t, t')\right.$$

$$\times \phi_{n'}\left(v'_z + \frac{e}{m}(A_z(t) - A_z(t')), t'\right) - \Omega_{nn'}(v_z, v'_z; t, t')$$

$$\left. \times \phi_n\left(v_z + \frac{e}{m}(A_z(t) - A_z(t')), t'\right)\right\}, \tag{5.17a}$$

with

$$\Omega_{nn'}(v_z, v_z'; t, t') = \frac{2}{\hbar^2} \mathrm{Re} \sum_q \sum_{\eta=-1,+1} \delta_{v_z, v_z'+(\eta\hbar q_z/m)} |J_{nn'}(q_x, q_y)|^2 |C(q)|^2 \left(N_q + \frac{1}{2} + \frac{\eta}{2}\right)$$
$$\times \exp\left\{-\frac{\mathrm{i}}{\hbar} \int_{t'}^{t} \mathrm{d}\tau \left(\epsilon_{n'}\left(\frac{mv_z' + e(A_z(t) - A_z(\tau))}{\hbar}\right) - \epsilon_n\left(\frac{mv_z + e(A_z(t) - A_z(\tau))}{\hbar}\right) + \eta\hbar\omega_q\right)\right\}. \quad (5.17b)$$

We underline that this equation is valid for a free electron gas submitted to uniform and parallel electric and magnetic fields, when only the electric field is possibly time dependent. The electric current density can be calculated according to the formula

$$J_z = \frac{e}{\Omega} \sum_{nK_y v_z} v_z \phi_n(v_z, t). \quad (5.18)$$

5.2. *Crossed fields configuration*

We turn our attention to the static case when the electric field is parallel to the x-axis and the magnetic field is along the z-axis. This problem has been explored many times[7]) by using the most convenient gauge which is

$$\text{Gauge } \mathcal{J}_B\text{: } \phi(r, t) = -eEx; \quad A = (0, Bx, 0). \quad (5.19)$$

In this gauge, the electron Hamiltonian is simply

$$H = \frac{1}{2m}(p_x^2 + (p_y - eBx)^2 + p_z^2) - eEx. \quad (5.20)$$

Its eigenstates $|\mu\rangle$ and its eigenvalues ϵ_μ are well known and the E.D.F.

$$f_\mu(t) = \langle \mu | \mathfrak{f}(t) | \mu \rangle \quad (5.21)$$

obeys the equation

$$\frac{\partial}{\partial t} f_\mu(t) = \int_{-\infty}^{t} \mathrm{d}t' \sum_{\mu'} \{W_{\mu'\mu}(t-t') f_{\mu'}(t') - W_{\mu\mu'}(t-t') f_\mu(t')\}, \quad (5.22a)$$

where

$$W_{\mu\mu'}(t-t') = \frac{2}{\hbar^2} \mathrm{Re} \sum_q \sum_{\eta=-1,+1} |\langle \mu | \chi_{\eta_q} | \mu' \rangle|^2 |C(q)|^2 \left(N_q + \frac{1}{2} + \frac{\eta}{2}\right)$$
$$\times \exp\left\{-\frac{\mathrm{i}}{\hbar}(\epsilon_\mu' - \epsilon_\mu + \eta\hbar\omega_q)(t-t')\right\}. \quad (5.22b)$$

The effect of the electric field on the collisions is entirely included in the expression of the eigenenergies ϵ_μ, in a way which is the simplest of all the cases studied here. Due to this relative simplicity, we have been able to solve under particular conditions the integral equation (5.22) (see for instance ref. 8). We can also notice that the stationary state corresponds here to the condition $\partial f_\mu(t)/\partial t = 0$, although there is no drift term in the l.h.s. of the transport equation (5.22).

6. Conclusion

We derived the evolution equation for the distribution function of electrons interacting with a phonon bath in three different physical situations:

(i) free electrons in the presence of a spatially uniform, but possibly time-dependent electric field,

(ii) Bloch electrons interacting with an electric field of the same type and finally

(iii) free electrons submitted to an electric field of the type described above and equally to a uniform and static magnetic field, parallel to the electric field.

The electron-phonon interaction was taken into account only at the lowest order, but there was no restriction on the intensity of the applied fields. The calculations were made simple owing to the choice of a vector-potential gauge to describe the electric field. For the Bloch electrons for instance, we introduced two distribution functions, firstly the distribution $f_\nu(\boldsymbol{K}, t)$ in the eigenstates of the electron Hamiltonian in the presence both of a periodic potential and of the electric field, and then the distribution function $\phi_\nu(\boldsymbol{k}, t)$ in the usual Bloch states, which deduces from $f_\nu(\boldsymbol{K}, t)$ by a gauge transformation.

The equation for $f_\nu(\boldsymbol{K}, t)$ is apparently much simpler than the transport equation for $\phi_\nu(\boldsymbol{k}, t)$. There is no drift term in the left-hand side and the $\boldsymbol{K}$-dependence of the collision term is very simple. However this equation must be handled with some care since for instance the stationary regime induced by a static electric field does not correspond to the condition $\partial f_\nu(\boldsymbol{K}, t)/\partial t = 0$.

On the other hand, the transport equation for $\phi_\nu(\boldsymbol{k}, t)$ contains a drift term in the left-hand side, and the collision integral involves distribution functions which, strictly speaking, depend on modified $\boldsymbol{k}$-vectors and have to be coarse-grained in $\boldsymbol{k}$-space in order to recover the usual $\boldsymbol{k}$-dependence. The stationary regime corresponds here to the standard condition $\partial\phi_\nu(\boldsymbol{k}, t)/\partial t = 0$.

In both formulations, the transition probabilities in the collision term do depend on the electric field: this dependence constitutes the intra-collisional-field-effect (I.C.F.E.). The existence of this effect has thus been established very simply in the three different physical situations quoted at the beginning of this section: free electrons, Bloch electrons and free electrons in the presence of a magnetic field.

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Appendix

Calculation of the product $P = \langle \nu \boldsymbol{K}|\chi_q|\nu \boldsymbol{K}'\rangle\langle \nu \boldsymbol{K}'|\chi_q^{\dagger}|\nu \boldsymbol{K}''\rangle$

Let us omit for the moment the band index ν. We obtain, from eq. (4.5),

$$P = \Omega^{-2}\left(\int \mathrm{d}\boldsymbol{r} w_{\boldsymbol{K}}^{*}(\boldsymbol{r}) \exp(-\mathrm{i}\boldsymbol{K}\cdot\boldsymbol{r}) \exp(\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{r}) w_{\boldsymbol{K}'}(\boldsymbol{r}) \exp(\mathrm{i}\boldsymbol{K}'\cdot\boldsymbol{r})\right)$$
$$\times \left(\int \mathrm{d}\boldsymbol{r} w_{\boldsymbol{K}'}^{*}(\boldsymbol{r}) \exp(-\mathrm{i}\boldsymbol{K}'\cdot\boldsymbol{r}) \exp(-\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{r}) w_{\boldsymbol{K}''}(t) \exp(\mathrm{i}\boldsymbol{K}''\cdot\boldsymbol{r})\right). \tag{A.1}$$

Since the functions $w_{\boldsymbol{K}}(\boldsymbol{r})$ are periodic we get, if c is the volume of the unit cell

$$P = \sum_{g_1}\sum_{g_2} \delta_{\boldsymbol{K}'+\boldsymbol{q}-\boldsymbol{K},\boldsymbol{g}_1}\delta_{\boldsymbol{K}''-\boldsymbol{q}-\boldsymbol{K}',\boldsymbol{g}_2}\frac{1}{c}\int_c \mathrm{d}\boldsymbol{r} w_{\boldsymbol{K}}^{*}(\boldsymbol{r}) w_{\boldsymbol{K}-\boldsymbol{q}+\boldsymbol{g}_1}(\boldsymbol{r}) \exp(\mathrm{i}\boldsymbol{g}_1\cdot\boldsymbol{r})$$
$$\times\frac{1}{c}\int_c \mathrm{d}\boldsymbol{r}' w_{\boldsymbol{K}-\boldsymbol{q}+\boldsymbol{g}_1}^{*}(\boldsymbol{r}') w_{\boldsymbol{K}+\boldsymbol{g}_1+\boldsymbol{g}_2}(\boldsymbol{r}') \exp(\mathrm{i}\boldsymbol{g}_2\cdot\boldsymbol{r}'), \tag{A.2}$$

where $\boldsymbol{g}_1$ and $\boldsymbol{g}_2$ are reciprocal lattice vectors and $\boldsymbol{K}$, $\boldsymbol{K}'$ and $\boldsymbol{K}''$ belong to the first Brillouin zone. The two delta symbols impose

$$\boldsymbol{K}'' - \boldsymbol{K} = \boldsymbol{g}_1 + \boldsymbol{g}_2. \tag{A.3}$$

Since $\boldsymbol{K}$ and $\boldsymbol{K}''$ belong both to the first Brillouin zone, this is only possible if

$$\boldsymbol{g}_1 + \boldsymbol{g}_2 = 0, \quad \text{i.e. } \boldsymbol{K}'' - \boldsymbol{K} = 0. \tag{A.4}$$

We get finally, after restablishing the band index ν:

$$P = \delta_{\boldsymbol{K},\boldsymbol{K}''}|\langle \nu\boldsymbol{K}|\chi_q|\nu\boldsymbol{K}'\rangle|^2 = \delta_{\boldsymbol{K},\boldsymbol{K}''}\sum_{g_1}\delta_{\boldsymbol{K}'-\boldsymbol{K}+\boldsymbol{q},\boldsymbol{g}_1}\left|\frac{1}{c}\int_c \mathrm{d}\boldsymbol{r} w_{\nu\boldsymbol{K}}^{*}(\boldsymbol{r}) w_{\nu,\boldsymbol{K}-\boldsymbol{q}}(\boldsymbol{r})\right|^2. \tag{A.5}$$

(We used the property

$$w_{\mathbf{K}+\mathbf{g}}(\boldsymbol{r})\exp(\mathrm{i}\mathbf{g}\cdot\boldsymbol{r}) = w_{\mathbf{K}}(\boldsymbol{r}).) \tag{A.6}$$

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