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A CONVENIENT GAUGE TREATMENT OF THE HIGH ELECTRIC FIELD ELECTRON DISTRIBUTION FUNCTION

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Résumé.- Grâce à un choix convenable de jauge pour le champ électrique uniforme appliqué, on établit très simplement des équations d'évolution pour les fonctions de distribution d'électrons chauds (électrons de Bloch ou électrons en présence de champ magnétique); on discute l'influence du champ électrique sur le terme de collision des équations de transport obtenues.

Abstract.- Owing to a convenient gauge choice for the uniform applied electric field, we establish very simply evolution equations for the hot electrons distribution functions (Bloch electrons or electrons in the presence of a magnetic field); we discuss the intra-collisional-field-effect in the different transport equations we derive.

I. INTRODUCTION.

For a long time the theory of electrons distribution functions (E.D.F.) had restricted its aim to describing the effect of an electric field on the drift motion of the electrons. I.B. Levinson [1] seems to have been the first to recognize the influence of an electric field on the electron-phonon collisions in solids. J.R. Barker [2] in collaboration with D.K. Ferry has already studied this phenomenon known since then as the intra-collisional-field-effect (I.C.F.E.). Their studies concerned essentially free electrons submitted to an electric field. We propose here a particularly simple method, well-suited to the derivation of the I.C.F.E. in the case of Bloch electrons. The simplicity of the calculations lies in the choice of the most convenient gauge describing the electric field. With this gauge choice it is possible to diagonalize the Hamiltonian associated with a Bloch electron submitted to a spatially uniform, time-dependent electric field, without any reference to Airy functions. We shall finally obtain two distinct evolution equations for two E.D.F. and discuss them in details. We shall also examine very briefly the case of free electrons submitted to parallel electric and magnetic fields.

II. QUANTUM BACKGROUND.

Let us consider a gas of independent electrons moving in applied electric and magnetic fields and in a periodic lattice potential $V(\mathbf{r})$. These electrons also interact with phonons assumed to be in thermal equilibrium. The total Hamiltonian is $H(t) = H(t) + H_p + H_{e-p}$ ($H(t)$ : electron Hamiltonian in the presence of the applied fields; $H_p$ : phonons Hamiltonian; $H_{e-p}$ : electron-phonon interaction Hamiltonian).
I.B. Levinson has established \[1\] that the electron density matrix \( \hat{f}(t) \) obeys the following equation valid at the lowest order in the electron-phonon coupling:

\[
i \hat{H} \frac{\partial}{\partial t} \hat{f}(t) - [\hat{H}(t), \hat{f}(t)] = \hat{C} \{ \hat{f}(t) \}
\]  

(1)

where \( \hat{C} \) is the collision operator, defined by:

\[
\hat{C} \{ \hat{f}(t) \} = -i \hbar \sum_q \langle C(q) \rangle^2 \left( N_{q+q} \right) \int_{-\infty}^{t} dt' \ e^{-i \omega_q (t-t')} \]

\[
\chi^+_q \exp \left(-\frac{i}{\hbar} \int_{t'}^{t} \hat{H}(\tau) d\tau \right) \chi^+_q \hat{f}(t') \exp \left( \frac{i}{\hbar} \int_{t'}^{t} \hat{H}(\tau) d\tau \right) + \text{Herm. Adj.}
\]

\[+ \text{ terms with } (N_{q+q}) \rightarrow (N_{q'-q}) , \omega_q \rightarrow \omega_{q'} , q \rightarrow -q .
\]

\( \hat{C}(\hat{q}) \) depends on 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 \( \chi^+_q = \exp(i \hat{q} \cdot \hat{r}) \). The I.C.F.E. appears simply in eq. (1') through the factors \( \exp(\frac{i}{\hbar} \int_{t'}^{t} \hat{H}(\tau) d\tau) \), where \( \hat{H}(t) \) includes the electric field.

### III. EVOLUTION EQUATION OF THE E.D.F. OF BLOCH ELECTRONS.

We now treat the special case of Bloch electrons. We shall assume for the sake of simplicity that we neglect interband transitions; thus the electrons always remain in the same band \( v \) and our purpose is to determine their E.D.F.

1) **Gauge choice and basis states.**— When we apply a uniform electric field \( \hat{E}(t) \), we do not change the periodicity of the potential \( V(r) \) acting on an electron in a crystal. This symmetry property appears clearly when we use the following gauge to describe the electric field \( \hat{E}(t) : \hat{A}(t) = -\int_0^t \hat{E}(\tau) d\tau \). With such a gauge choice, the electron Hamiltonian is simply:

\[
\hat{H}(t) = \frac{(\hat{r} - e \hat{A}(t))^2}{2m} + V(\hat{r})
\]  

(2)

There is a relation between \( \hat{H}(t) \) and the electron Hamiltonian in the absence of the electric field:

\[
\hat{H}_0 = \frac{\hat{p}^2}{2m} + V(\hat{r}) \quad \text{with} \quad \hat{H}_0 |\hat{k}\rangle = \varepsilon(\hat{k}) |\hat{k}\rangle
\]  

(3)

with \( |\hat{k}\rangle \) and \( \varepsilon(\hat{k}) \) are respectively the usual Bloch states and energy bands expressions. That relation is simply:

\[
\hat{H}(t) = T \hat{H}_0 T^+ \quad \text{where} \quad T = \exp(i \frac{e}{\hbar} \hat{r} \cdot \hat{A}(t))
\]  

(4)

\( T \) is none other than the unitary operator corresponding to the gauge transformation \( \hat{H}(t) \rightarrow \hat{\mathcal{H}} = \hat{p}^2/2m + V(\hat{r}) - e \hat{E} \cdot \hat{r} \) ( \( \hat{\mathcal{H}} \) is the Hamiltonian in the ordinary scalar potential gauge). Thus \( \hat{H}(t) \) has Bloch type eigenstates \( |\hat{k}\rangle \) such that:
\( H(t) |\tilde{k}\rangle = E(\tilde{k}) |\tilde{k}\rangle \) with \( <\tilde{\gamma}|\tilde{k}\rangle = e^{i\tilde{k}\cdot r} \psi_{\tilde{k}}(\tilde{r}) \) (7)

(\( \psi_{\tilde{k}}(\tilde{r}) \) is the periodic part of the Bloch function). From eqs. (4)–(7) we deduce that

\[ |\tilde{k}\rangle = T |\tilde{k}\rangle \] (8) and \( E(\tilde{k}) = e(\tilde{k}) \) (8')

with \( \tilde{k} = \tilde{k} + \frac{e}{\hbar} A(t) \) (9)

In short, if we introduce the vector \( \tilde{k}(t) = \tilde{k} - \frac{e}{\hbar} A(t) \) and insert the band index \( \nu \) omitted until now, we find a most useful equation for what follows:

\[ H(t) |\nu\tilde{k}\rangle = \epsilon_{\nu} (\tilde{k}(t)) |\nu\tilde{k}\rangle \] (10)

2) Evolution equations. It is straightforward to derive from eqs. (1) and (1') the evolution equation of the E.D.F. in the eigenstates of \( H(t) \). Such an E.D.F. is defined by

\[ f_{\nu}(\tilde{k}, t) = \langle \nu\tilde{k} | f(t) |\nu\tilde{k}\rangle \] (11)

When we compute the diagonal elements of the two members of eq. (1), the left-hand-side gives simply \( \frac{\partial}{\partial t} f_{\nu}(\tilde{k}, t) \); for the right-hand-side we find expressions such as:

\[ C_{\nu}(\tilde{k}) = \langle \nu\tilde{k} | \sum_{q} e^{i\tilde{k}\cdot \tilde{r}(t)} \int_{t'}^{t} H(\tau) \, d\tau \langle \tilde{r}(t) | f(t') \rangle \exp\left( \frac{i}{\hbar} \int_{t'}^{t} H(\tau) \, d\tau \right) |\nu\tilde{k}\rangle \]

Since we assumed that the electrons always remain within the same energy band \( \nu \), we obtain:

\[ \frac{\partial}{\partial t} f_{\nu}(\tilde{k}, t) = \int_{t'}^{t} dt' \sum_{\tilde{k}'} \left\{ P_{\nu}(\tilde{k}', \tilde{k}; t, t') f_{\nu}(\tilde{k}', t') - P_{\nu}(\tilde{k}, \tilde{k}'; t, t') f_{\nu}(\tilde{k}, t) \right\} \] (12)

where

\[ P_{\nu}(\tilde{k}, \tilde{k}'; t, t') = \frac{2}{\hbar} \text{Re} \sum_{\nu} \sum_{\eta = -1, +1} |\langle \nu\tilde{k}| \chi_{\nu}^{\eta} |\nu\tilde{k}'\rangle|^{2} |C(\nu)_{\eta}|^{2} \left( \frac{N-\frac{1}{2} + \frac{\eta}{2}}{2} \right) \exp\left( \frac{i}{\hbar} \int_{t'}^{t} d\tau \left( \epsilon_{\nu}(\tilde{k} - \frac{\eta}{\hbar} \tilde{A}(\tau)) - \epsilon_{\nu}(\tilde{k} - \frac{\eta}{\hbar} \tilde{A}(\tau)) + \eta \omega_{\nu} \right) \right) \] (12')

The two last equations call for many comments:

(i) There is no drift term proportional to \( \tilde{E}(t) \) in the left-hand-side of eq. (12); the whole effect of the electric field is included in the collision term, at the right-hand-side;

(ii) The collision term is non-Markoffian;

(iii) Even in the case of a static electric field, we cannot rewrite the collision term under the form of a convolution product since the probabilities \( P_{\nu}(\tilde{k}, \tilde{k}'; t, t') \) are not functions of the time difference \( (t-t') \); this implies in turn that we cannot find by the usual technics a Markoffian equation for \( f_{\nu}(\tilde{k}, t) \) in the
asymptotic limit \((t \to \infty)\);

(iv) The stationary state in a static electric field \(\overrightarrow{E}_0\) does not correspond to the condition that one could expect \(\frac{\partial}{\partial t} f_\nu(\overrightarrow{k},t) = 0\); we shall return to this point later, in more detail;

(v) We can transform eqs. (12) and (12') in order to obtain the E.D.F. in the usual Bloch eigenstates \(|\nu\overrightarrow{k}\rangle\) of the Hamiltonian \(H_0\).

In order to understand this last point, we notice that eqs. (8) and (11) give

\[
f_\nu(\overrightarrow{k},t) = \langle \nu\overrightarrow{k} | \hat{f}(t) | \nu\overrightarrow{k}\rangle = \langle \nu\overrightarrow{k} | T^{+}\overrightarrow{\hat{f}}(t) T | \nu\overrightarrow{k}\rangle = \langle \nu\overrightarrow{k} | \hat{f}(t) | \nu\overrightarrow{k}\rangle
\]

The operator \(T^{+}\overrightarrow{\hat{f}}(t) T\) represents the density matrix \(f_\nu\) of the electrons when the scalar potential gauge is used, and thus \(\phi_\nu(\overrightarrow{k},t) = \langle \nu\overrightarrow{k} | \hat{f}(t) | \nu\overrightarrow{k}\rangle\) is the E.D.F. in the usual Bloch eigenstates of the Hamiltonian \(H_0\). From eqs. (9) and (11) we get immediately:

\[
f_\nu(\overrightarrow{k},t) = \phi_\nu(\overrightarrow{k},t) \tag{13}
\]

\[
\frac{\partial}{\partial t} f_\nu(\overrightarrow{k},t) = \frac{\partial}{\partial t} \phi_\nu(\overrightarrow{k},t) + \frac{e}{\hbar} \cdot \overrightarrow{\nabla}_\overrightarrow{k} \phi_\nu(\overrightarrow{k},t) \tag{14}
\]

\[
f_\nu(\overrightarrow{k},t') = \phi_\nu(\overrightarrow{k} + \frac{e}{\hbar} (\overrightarrow{A}(t)-\overrightarrow{A}(t')),t') \tag{15}
\]

\[
\epsilon_\nu(\overrightarrow{k} - \frac{e}{\hbar} \overrightarrow{A}(t)) = \epsilon_\nu(\overrightarrow{k} + \frac{e}{\hbar} (\overrightarrow{A}(t)-\overrightarrow{A}(t))) \tag{16}
\]

Inserting eqs. (14) to (17) into eqs. (12) and (12'), we finally obtain the transport equation for the E.D.F. in the usual Bloch states

\[
\frac{\partial}{\partial t} \phi_\nu(\overrightarrow{k},t) + \frac{e}{\hbar} \cdot \overrightarrow{\nabla}_\overrightarrow{k} \phi_\nu(\overrightarrow{k},t) = \tag{18}
\]

\[
\int_{-\infty}^{t} dt' \sum_{\overrightarrow{k}'} \{ \Pi_\nu(\overrightarrow{k}',\overrightarrow{k},t,t') \phi_\nu(\overrightarrow{k}'+\frac{e}{\hbar} (\overrightarrow{A}(t)-\overrightarrow{A}(t')),t')
\]

\[
- \Pi_\nu(\overrightarrow{k},\overrightarrow{k}',t,t') \phi_\nu(\overrightarrow{k}'+\frac{e}{\hbar} (\overrightarrow{A}(t)-\overrightarrow{A}(t')),t') \}
\]

with

\[
\Pi_\nu(\overrightarrow{k},\overrightarrow{k}',t,t') = \frac{2}{\hbar^2} \text{Re} \sum_{\overrightarrow{q}} \sum_{\eta=-1,1} \langle \nu\overrightarrow{k} | \chi_{\eta\overrightarrow{q}} | \nu\overrightarrow{k}'\rangle^2 |c_{\overrightarrow{q}}^*|^2 (\eta \overrightarrow{q} + \frac{1}{2}) \tag{18'}
\]

\[
\exp\left(\frac{i}{\hbar} \int_{t'}^{t} dt \left( \epsilon_\nu(\overrightarrow{k}'+\frac{e}{\hbar} (\overrightarrow{A}(t)-\overrightarrow{A}(t'))) - \epsilon_\nu(\overrightarrow{k}+\frac{e}{\hbar} (\overrightarrow{A}(t)-\overrightarrow{A}(t'))) + \eta \overrightarrow{q} \overrightarrow{a} \right) \right)
\]

This transport equation, when written for free electrons, instead of Bloch electrons, in an applied electric field, becomes identical to that of ref. [22]. It is valid at the lowest order in the electron-phonon coupling, whatever the details of the band structure. We recover in eq. (18) the usual drift term. Due to factors such as \(\frac{e}{\hbar} (\overrightarrow{A}(t)-\overrightarrow{A}(t'))\) in the argument of \(\phi_\nu\), the non-Markoffian collision term never appears as a convolution product. The dependence on the electric field in the transition probabilities \(\Pi_\nu\) constitutes the intra-collisional-field-effect (I.C.F.E.).
The electric current density can be expressed through the E.D.F.:

\[ \mathbf{J} = e \sum_{K} \frac{1}{\Omega} \psi_\nu^* (\mathbf{K} - \frac{e}{\hbar} \mathbf{A}(t)) \psi_\nu (\mathbf{K}, t) = e \sum_{K} \frac{1}{\Omega} \psi_\nu^* (\mathbf{K}) \psi_\nu (\mathbf{K}, t) \]  \hspace{1cm} (19)

(\Omega is the volume of the sample). When we consider the stationary regime induced by a static electric field \( \mathbf{E}_0 \), it is clear that the E.D.F. \( \phi_\nu (\mathbf{K}, t) \) reaches a time-independent value that we label \( \phi_\nu (\mathbf{K}) \). From eqs. (9) and (14) we deduce that

\[ \lim_{t \to \infty} f_\nu (\mathbf{K}, t) = \phi_\nu (\mathbf{K} + \frac{e}{\hbar} \mathbf{E}_0 t) \] \hspace{1cm} (20)

This last result shows, as we already remarked, that in the stationary state, \( f_\nu \) depends on time through \( \mathbf{K} + \frac{e}{\hbar} \mathbf{E}_0 t \).

IV. FREE ELECTRONS IN PRESENCE OF UNIFORM PARALLEL ELECTRIC AND MAGNETIC FIELDS.

We limit ourselves to the main features of the calculations which are very similar to the Bloch case. The convenient gauge is now: \( A_x = 0, A_y = Bx, A_z = - \int_0^t \mathbf{E}(t) \, dt \). Then \( \mathbf{E}(t) \) and \( \mathbf{B} \) are both parallel to the \( z \) axis and uniform. With this gauge the electron Hamiltonian writes:

\[ H(t) = \frac{\left( \mathbf{p} - e \mathbf{A}(t) \right)^2}{2m} \]  \hspace{1cm} (21)

and its symmetry properties are exactly the same as in the absence of the electric field. It is easy to verify that the Landau states \( |nK_y, K_z > \) are the eigenstates of \( H(t) \) and that

\[ H(t) \left| nK_y, K_z > \right. = \varepsilon_n (K_z - \frac{e}{\hbar} A_z (t)) \left| nK_y, K_z > \right. \] \hspace{1cm} (22)

where

\[ \varepsilon_n (K_z - \frac{e}{\hbar} A_z (t)) = (n + \frac{1}{2}) \omega_c + \frac{(K_z - e A_z (t))^2}{2m} \] \hspace{1cm} and \( \omega_c = \frac{|e|B}{m} \) \hspace{1cm} (22')

Again eq. (22) is the key to obtaining the evolution equation for the E.D.F. in the Landau states; from it we immediately deduce a transport equation for the velocity distribution function. The structure of these two equations looks very similar to that of eqs. (12)-(12') and (18)-(18'); all the comments which follow them can be repeated.

V. CONCLUSION.

We derived equations for the distribution functions of Bloch electrons interacting with a phonon bath and a uniform time-dependent electric field. The electron-phonon interaction was treated at the second order and the electric field at all orders. Two E.D.F. have been explored: the first one, \( f_\nu (\mathbf{K}, t) \), in the eigenstates of the Hamiltonian \( H(t) \) of an electron including both the effects of the periodic potential and of the electric field; the second one, \( \phi_\nu (\mathbf{K}, t) \), in the usual Bloch states, deduced from \( f_\nu (\mathbf{K}, t) \) by a gauge transformation. The evolution equation
for $f_v(\vec{K},t)$ seems much simpler than the transport equation for $\phi_v(k,t)$. There is no drift term in its left-hand-side and the electric field dependence of the collision term seems less complex. However this equation must be handled with care since for instance the stationary regime induced by a static electric field does not correspond to the condition $\frac{\partial}{\partial t} f_v(\vec{K},t) = 0$. The technique is easily extended to the case where free electrons interact not only with an electric field but also with a parallel magnetic field.

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