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Longitudinal Conductivity of Metals for Inter- and Intraband Transitions in a Magnetic Field

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Expressions for the longitudinal conductivity of metals in a magnetic field are obtained using a set of wave functions consistent with the effective-mass energies and following a method essentially the same as that employed by Dresselhaus and Dresselhaus. It is found that the resulting expressions do not conform to the physical results.

A calculation of the longitudinal conductivity of metals in a magnetic field is presented by Dresselhaus and Dresselhaus[1] (hereafter referred to as DD), building on an earlier work by Mattis and Dresselhaus.[2] The approach of DD to the problem is based on a density-matrix technique originally developed by Karplus and Schwinger.[3] It is important to note that DD did not use a consistent set of energies and wave functions. The energies used were the well-known effective-mass energies, while the wave functions were the lowest-order wave functions of Luttinger and Kohn (LK).[4] These are known not to be compatible (see, e.g., Smith *et al.*[5]). In an attempt to compensate for this and to obtain physically sensible results, DD replaced in an *ad hoc* way the electron mass m_0 by the effective mass for the band m_n^* wherever certain matrix elements of momentum were encountered. In this paper, a set of wave functions consistent with the effective-mass energies is used to treat the same problem. A variational-perturbative technique is employed to find perturbed eigenfunctions and energy levels for the case of Bloch electrons in an external magnetic field, using LK functions as zero-order wave functions. The physical system to which the present calculations are applied is the same as that considered by DD (the same notation as that used by DD will be used throughout this paper unless otherwise indicated).

We take the state vectors $|nl\vec{q}\rangle$ for the static problem, i.e., when the rf field is switched off, to satisfy to first order

$$\mathcal{H}_0\,|nl\vec{q}\rangle=\mathcal{E}_n^l(\vec{q})\,|nl\vec{q}\rangle ,$$

where

$$\mathcal{E}_n^l(\vec{q})=\hbar^2q_x^{\,2}/2m_n^*+\hbar\omega_c^{(n)}\,(l+\tfrac{1}{2})+\mathcal{E}_n(0)$$

are the energy eigenvalues in the effective-mass approximation (they are consistent with the f-sum rule), and the $|nl\vec{q}\rangle$, constituting a complete orthonormal set to first order, are given in terms of the $|nl\vec{q})$ (the LK zero-order state vectors) by

$$|nl\vec{q}\rangle=|nl\vec{q})+\mathop{\mathbf{S}'}_{n'l'q'}\frac{|n'l'\vec{q}')(n'l'\vec{q}'\,|\,\mathcal{H}_0\,|nl\vec{q})}{\mathcal{E}_n^l(\vec{q})-\mathcal{E}_{n'}^{l'}(\vec{q}')} .$$

The symbol $\mathbf{S}$ refers to the summation over discrete indices and integration over continuous ones. The prime over the $\mathbf{S}$ indicates that the term with n', l', $\vec{q}'=n$, l, $\vec{q}$ is omitted in the summation.

The main concern is the calculation of the Fourier transform of the mean value of the current density

$$\langle\vec{j}(\vec{\kappa})\rangle=\frac{(2\pi)^{-3/2}e}{m}\sum_{1,2,3}\langle 1\,|\,\rho\,|\,2\rangle\langle 2\,|\,e^{i\vec{\kappa}\cdot\vec{r}}\,|\,3\rangle \times\langle 3\,|\,\vec{p}-(e/c)\vec{A}\,|\,1\rangle ,$$

where $|1\rangle$ stands for $|n_1,l_1,\vec{q}_1\rangle$, etc. In order to evaluate explicitly the expression for $\langle\vec{j}(\vec{\kappa})\rangle$ one needs the various matrix elements appearing in it. Explicit expressions for these are given by DD.

There are, however, some corrections needed. The matrix elements $\langle 1|\vec{p}|2\rangle$ are formally the same as Eq. (28) of DD, with $|)$ replaced by $|\rangle$. The corrected matrix elements of p_x are

$$(1|p_x|2)=(2\pi)^2\,\delta_{l_1l_2}\,\delta(\vec{q}_1-\vec{q}_2)\,(n_1l_2\vec{q}_2|p_x|n_2l_2\vec{q}_2)$$

and

$$(1|p_x|1)=(2\pi)^{-2}\hbar q_x\,.$$

The f-sum rule [Eq. (37) of DD] should be given as

$$\frac{2(2\pi)^4}{m_0}\sum_{n'\neq n}\frac{|(nl\vec{q}_0|p_x|n'l\vec{q}_0)|^2}{\mathcal{E}^l_{n'}(\vec{q}_0)-\mathcal{E}^l_n(\vec{q}_0)} =1-\frac{m_0}{\hbar}\left(\frac{\partial^2\mathcal{E}^l_n(\vec{q})}{\partial q_x^2}\right)_{\vec{q}_0}\,.$$

Also used in the calculation of the intraband term are the diagonal matrix elements of p_x with respect to $|\rangle$; they are given by

$$\langle 1|p_x|1\rangle=\frac{m_0}{(2\pi)^2\hbar}\left(\frac{\partial\mathcal{E}^l_n(q)}{\partial q_x}\right)_{\vec{q}_1}\,.$$

In the calculation many terms appear which would contribute to the interband terms were they not to vanish according to the symmetry requirements. In particular, it is assumed that Bloch wave functions at the bottom of the band are nondegenerate apart from time-reversal degeneracy, and that the periodic potential $V_p(\vec{r})$ is invariant under inversion. Then terms such as $(n_3l_2\vec{q}\,|p_x|n_1l_2\vec{q})(n_1l_1\vec{q}|p_x|\times n_2l_1\vec{q})(n_2l_1\vec{q}|\mathcal{H}_0|n_3l_2\vec{q})$ vanish due to the Bloch wave functions possessing a definite parity.

The results are expressed in terms of a longitudinal conductivity $\sigma_{xx}(\kappa_z)$, which is related to $\langle\vec{j}(\vec{k})\rangle$ as follows (since $\vec{E}$ depends only on the z coordinate):

$$\langle\vec{j}(\vec{k})\rangle_x=\pi\delta(\kappa_x)\,\delta(\kappa_y)\,E_x(\kappa_z)\,e^{i\omega t}\,\sigma_{xx}(\kappa_z).$$

The σ_{xx} may be separated into inter- and intraband terms:

$$\sigma^{\text{intra}}_{xx}=\frac{e^2}{2\pi^2 i\lambda^2}\sum_{n,l,l'}\frac{1}{m_0}\left\{|J_{ll'}(\lambda^2\kappa_z)|^2\left[\frac{m^*_n}{m_0}\frac{\omega-i/\tau_{nn}}{(\omega-i/\tau_{nn})^2-[\omega_c^{(n)}(l-l')]^2}\right.\right.$$
$$\left.\left.+\frac{1}{\omega}\left(\frac{m_0}{m^*_n}-\frac{m^*_n}{m_0}\right)+\left(\frac{m^*_n}{m_0}-1\right)\left(\frac{1}{\omega}-\frac{1}{\omega-i/\tau_{nn}+\omega_c^{(n)}(l-l')}\right)(1+\delta_{ll'})\right]\right\}\int dq_x\,f_0[\mathcal{E}^l_n(q_x)]$$

and

$$\sigma^{\text{inter}}_{xx}=\frac{e^2\hbar}{2\pi^2 i\lambda^2 m_0^2}\sum_{\substack{n,n',l,l'\\ n'\neq n}}|J_{ll'}(\lambda^2\kappa_z)|^2\int dq_x\,\frac{f_0[\mathcal{E}^l_n(q_x)]-f_0[\mathcal{E}^{l'}_n(q_x)]}{\mathcal{E}^l_n(q_x)-\mathcal{E}^{l'}_{n'}(q_x)}$$
$$\times(2\pi)^4|(nl\vec{q}|p_x|n'l\vec{q})|^2\left(\frac{\mathcal{E}^{l'}_n(q_x)-\mathcal{E}^l_n(q_x)}{\hbar\omega[\mathcal{E}^l_n(q_x)-\mathcal{E}^l_{n'}(q_x)]}-\frac{1}{\hbar(\omega-i/\tau_{nn'})+\mathcal{E}^l_n(q_x)-\mathcal{E}^l_{n'}(q_x)}\right),$$

where

$$J_{ll'}(\lambda^2\kappa_z)=\int dy\,\phi^*_l(y)\,\phi_{l'}(y-\lambda^2\kappa_z).$$

It is easily seen from the expression for $\sigma^{\text{intra}}_{xx}$ that Ohm's law and the zero-field result of the Drude model for $V_p\neq 0$ are not recovered. This arises from the fact that in writing the expression for $\mathcal{E}^l_n(\vec{q})$ it is assumed that an effective mass is produced due to the coupling of the nth band to other bands, whereas if such a coupling exists, then the magnetic energy levels should be complicated expressions depending on coupling between all Landau levels in the nth band to all other Landau levels. This difficulty can be overcome by using magneto-translationally invariant wave functions.[6]

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