Electrical current and magnetic fields in conductors with mirror-isomeric structure

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A linear relation between the current and the magnetic field can exist in conductors with mirror-isomeric structure. An explicit expression is obtained for the corresponding tensor and some physical consequences of such a relation for the thermodynamic and electrical conductivities are discussed.

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Point groups of crystals, which occur in two mirror-isomeric (enantiomorphic) modifications, do not contain improper elements that transform a right-handed coordinate system into a left-handed one. In conductors with such symmetry, a linear relation is admissible between the electrical current density **j** and the magnetic field intensity $\mathbf{H}$: $j_\mu = \kappa_{\mu\nu} H_\nu$. The existence of such a relation, at first glance, contradicts energy considerations, if we are talking about macroscopic currents induced by the magnetic field. If, on the other hand, the current is fixed by an external source, then these considerations are no longer valid. This problem especially deserves discussion, since such a relation, as will be demonstrated below, indeed occurs due to the spin-orbital interaction.

We shall write the current density in the linear approximation in terms of the time-independent vector potential **A**, under the assumption that the substance is nonmagnetic ($\mathbf{H} \cong \mathbf{B}$, rot $\mathbf{A} = \mathbf{H}$, div $\mathbf{A} = 0$):

$$j_\mu(\mathbf{r}) = \int d^3r'\, Q_{\mu\nu}(\mathbf{r}, \mathbf{r}')\, A_\nu(\mathbf{r}') - \frac{e^2}{mc} n(\mathbf{r}) A_\mu(\mathbf{r}) . \tag{1}$$

The Fourier component of the kernel Q is

$$Q_{\mu\nu}(\mathbf{q},\mathbf{q}') = -\frac{e^2}{c} T \sum_n \sum_{\alpha,\beta} \int\int \frac{d^3k d^3k'}{(2\pi)^6} \frac{\int d^3r e^{-i\mathbf{qr}} \bar{\psi}_{\beta k'} \hat{v}_\mu \psi_{\alpha k} \int d^3r' e^{-i\mathbf{q}'\mathbf{r}'} \bar{\psi}_{\alpha k} \hat{v}_\nu \psi_{\beta k'}}{(i\epsilon_n + \zeta - \epsilon_{\alpha k})(i\epsilon_n + \zeta - \epsilon_{\beta k'})}. \tag{2}$$

Here α and β are the band indices, $\mathbf{k}$ and $\mathbf{k}'$ are the wave vectors in the Brillouin zone, T is the temperature, ζ is the chemical potential, and $\epsilon_n = (2n+1)\pi T$.[1] The problem reduces to transformation of matrix elements, in which $\psi_{\alpha k} = e^{i\mathbf{qr}} u_{\alpha k}$ are the eigenfunctions (2-component spinors) of the energy operator of an electron in a lattice in the absence of a field: $\mathscr{H}\psi_{\alpha k} = \epsilon_{\alpha k}\psi_{\alpha k}$, and $u_{\alpha k}$ are normalized to the unit cell $V_0 \hbar \hat{\mathbf{v}} = i[\mathscr{H},\mathbf{r}]$. Precise calculations[2] lead to the expression

$$\int d^3r e^{-i\mathbf{qr}} \bar{\psi}_{\beta k'} \hat{v}_\mu \psi_{\alpha k} = \frac{1}{\hbar} \left\{ \frac{\partial \epsilon_{\alpha k}}{\partial k_\mu} \int_{V_0} d^3r \bar{u}_{\beta k'} u_{\alpha k} + \sum_\gamma (\epsilon_{\alpha k} - \epsilon_{\gamma k}) a^\mu_{\alpha\gamma} \int_{V_0} d^3r \bar{u}_{\beta k'} u_{\gamma k} \right\} (2\pi)^3 \delta(\mathbf{k} - \mathbf{k}' - \mathbf{q}) \tag{3}$$

and analogously for the second matrix element. Thus, a single integration over $\mathbf{k}$ remains in (2), and $Q_{\mu\nu}(\mathbf{q},\mathbf{q}') = (2\pi)^3 \delta(\mathbf{q} - \mathbf{q}') Q_{\mu\nu}(\mathbf{q})$. The matrix vector $a^\mu_{\alpha\beta}$ is defined by the relation

$$a^\mu_{\alpha\beta}(\mathbf{k}) = \int_{V_0} d^3r \bar{u}_{\beta k} \frac{\partial u_{\alpha k}}{\partial k_\mu} \; ; \quad (a^\mu_{\beta\alpha})^* = -a^\mu_{\alpha\beta} . \tag{4}$$

Expanding $Q_{\mu\nu}(\mathbf{q})$ in a series in powers of $\mathbf{q}$ up to linear terms, we can verify that $Q_{\mu\nu}(0)$ cancels out the second term in (1). In calculating terms linear in $\mathbf{q}$, the following identity is used:

$$\frac{\partial a^\mu_{\alpha\beta}}{\partial k_\nu} - \frac{\partial a^\nu_{\alpha\beta}}{\partial k_\mu} = \sum_\gamma (a^\nu_{\alpha\gamma} a^\mu_{\gamma\beta} - a^\mu_{\alpha\gamma} a^\nu_{\gamma\beta}). \tag{5}$$

Elementary calculations lead to the simple result

$$j_\mu = -i\kappa e_{\mu\nu\lambda} q_\lambda A_\nu \; ; \quad \kappa = \frac{ie^2}{\hbar^2 c} \sum_\alpha \int \frac{d^3k}{(2\pi)^3} n_{\alpha k} (\vec{\nabla}_k \epsilon_{\alpha k} \, \mathrm{rot}_k \, \mathbf{a}_{\alpha\alpha}), \tag{6}$$

where $e_{\mu\nu\lambda}$ is the completely antisymmetrical unit tensor, $n_{\alpha k}$ are the Fermi occupation numbers, $\mathrm{rot}_k \mathbf{a}_{\alpha\alpha}$ is the curl of the diagonal element of matrix vector (4) in $\mathbf{k}$ space. An important (and rather unexpected) consequence of (6) is the fact that the relation between the current and the field is isotropic, in spite of the crystalline anisotropy,

$$\mathbf{j} = \kappa \mathbf{H}. \tag{7}$$

Since the coefficient κ is a pseudoscalar, both signs are equivalent and it can thus differ from zero only in the case of symmetry corresponding to enantiomorphism: isomers differ by the sign of κ. On the other hand, it is evident from (6), (4), and (5) that $\kappa \neq 0$ only if the representation, according to which $u_{\alpha k}$ transform, cannot be reduced to a real form. This case is realized for the symmetry in question when it is known that there is no inversion center and there is no degeneracy in the common point of the

Brillouin zone due to spin-orbit interaction. In addition, states with wave vectors **k** and $-\mathbf{k}$ transform into each other under time inversion (see, for example, Ref. 3).

We note that the structure of (6) ensures that there is no contribution from completely filled bands.

At this stage, we can only give a very rough estimate of the magnitude of the coefficient κ, which, just as the conductivity, has the dimension of frequency. Writing κ in accordance with (6) in the form $(e^2/\hbar c)\Omega$, where Ω is an atomic frequency ($\hbar^{-1}$ rydberg), it is not difficult, judging from what was said above, to see that the dimensionless factor is small due to the weakness of the spin-orbit interaction of the electron with the asymmetric part, relative to improper transformations, of the lattice potential. The nature of the temperature dependence of κ is clear from the fact that there must be a difference between the population of the states split by this interaction. Since (6) is thermodynamic in nature (in contrast to the conductivity), scattering plays a role only to the extent that it distorts the spectrum and the wave functions. For this reason, scattering does not lead to catastrophic effects and can be included using perturbation theory.

We shall now examine a cylindrical conductor with a cross-sectional radius ρ_0, closed into a ring with a large radius $R \gg \rho_0$ and placed along the axis of a toroidal solenoid, creating a longitudinal field H_0. If the current and field distributions inside the conductor are controlled by relation (7), then, solving the equation rot $\mathbf{H} = (4\pi\kappa/c)\mathbf{H}$ with the usual boundary conditions, we obtain the following expressions for the components of the field H_z along the axis of the cylinder and H_ϕ along the azimuth:

$$H_z = H_0 \frac{J_0(x)}{J_0(x_0)} \; ; \; H_\phi = \frac{\kappa}{|\kappa|} H_0 \frac{J_1(x)}{J_0(x_0)}, \quad \rho < \rho_0$$

$$H_z = H_0 \; ; \qquad H_\phi = \frac{\kappa}{|\kappa|} H_0 \frac{x_0}{x} \frac{J_1(x_0)}{J_0(x_0)}, \quad R \gg \rho > \rho_0, \tag{8}$$

where $J_n(x)$ are Bessel functions, $x = (4\pi\kappa/c)\rho$, and $x_0 = (4\pi\kappa/c)\rho_0$. The difference between the energies of this field distribution and the field in the absence of the conductor is

$$\frac{1}{8\pi} \int d^3r (H^2 - H_0^2) = V \frac{H_0^2}{8\pi} \left\{ 2 \left[\frac{J_1(x_0)}{J_0(x_0)} \right]^2 \ln \frac{R}{\rho_0} - \frac{J_2(x_0)}{J_0(x_0)} \right\} \tag{9}$$

(V is the volume of the conductor). As is evident, it consists of two parts: the first part, written with logarithmic accuracy, is the energy associated with the self-induction of the ring and the second part is the energy of the magnetic moment of the current j_ϕ in the field H_0. We note that the latter, for large values of X_0, is close to $H_0^2/8\pi$, as in the case of an ideal diamagnetic material. Because of the oscillating nature of $J_n(x_0)$, the expressions obtained are very sensitive to the geometrical factors. However, for our purposes, it is significant that in the example being studied this energy is positive and very large compared to the energy determined by the usually small susceptibility, χ. For this reason, it is natural that when the field is switched on, there must be some restructuring of the thermodynamic equilibrium state in the type of conductor being examined. As a result, there will be no macroscopic currents or high energy of the field associated with them. This especially concerns singly connected conductors. Since the energy density of the conductor has, aside from a part related to the susceptibility $-(1/2)\chi H^2$, a term corresponding to the current (7), $-(\kappa/2c)\mathbf{A}\cdot\mathbf{H}$, it would be reasonable to formulate the problem of the formation of a spatially modulated state.[1)] We hope to return in the future to a more detailed description of the structure of the state that arises. Here we only note that the energy scale of the restructuring is determined by the low susceptibility χ and is thus insignificant. For this reason, there must be an anomalous sensitivity to the alternating field.

The situation changes if the conductor characterized by a nonzero value of κ is connected into a circuit with an external current source. In this case, there is no *a priori* basis for "switching off" the current (7) and, in addition, an electric field $\mathbf{E}$ arises, so that $\mathbf{j}=\sigma\mathbf{E}+\kappa\mathbf{H}$. For a dc current, rot $\mathbf{E}=0$ and $\mathbf{E}$ is uniform along the conductor. In addition, the expression for the total current in the case of a cylindrical conductor in the presence of an external longitudinal magnetic field H_0 [the notation is the same as in (8)] is as follows:

$$I_z=\frac{c\rho_0}{2\kappa}\frac{J_1(x_0)}{J_0(x_0)}\left(\sigma E+\kappa H_0\right). \tag{10}$$

We see that the picture of the electrical conductivity differs sharply from the usual picture. Aside from the anomalous dependence on the external magnetic field, the effective conductivity oscillates as a function of x_0, which must also be manifested in the temperature behavior: in a fixed section, x_0 depends on T together with κ. By varying H_0 and x_0, it is possible to achieve a sharp decrease in E with a fixed current. Sections with negative conductivity, in which the stability of the static picture is lost, do exist. In addition, under conditions when the current is fixed, it may be expected, based on the requirement of minimum dissipation, that in sections where the effective conductivity is less than σ, the state corresponding to "switching-off" of the current (7) will be restructured. These characteristics should indeed be expected to appear in the region of values $x_0\sim 1$.

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