Anomalies in the conductivity of thin polycrystalline films in a distortion field

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This paper establishes the existence of quantum oscillations in the conductivity of a thin polycrystalline film under the action of a distortion field, using a model of the film based on the theory of bundle spaces and loop groups. In this model, the distortion 4-vector corresponds to the connectivity coefficient of the principal fibration, while the dislocation flux density tensor corresponds to the components of a curvature 2-form. The character of quantum corrections to the conductivity of a thin polycrystalline film is determined. It is shown that the frequency and amplitude of the oscillations is determined by the intensity of the distortion. From a geometric point of view, the anomalies described here are a consequence of a theorem regarding the transport of the connection of the principal fiber bundle.

In recent years there has been considerable interest in evaluating the usefulness of methods of differential geometry and topology in constructing models of disordered structure. In a number of papers[1–4] based on the theory of bundle spaces and loop groups[5] models of thin polycrystalline films were constructed which take into account the influence of the degree of ordering of the substructure on the kinetic characteristics. In these models a thin polycrystalline film is placed in correspondence with the principal bundle space $P(M,G)$, where P is a basis and G is the structural group of the fibration. In the present case this space has a rather simple structure: the basis is the space $R^4 \oplus v^\infty$, and $G = U(1)$. This construction is supplemented by an associated fibration $E(M,G,H,P)$, where the standard layer H is chosen to be a separable subspace of the Hilbert space. The set of intergrain boundaries is identified with a set of loops which can be reduced to a loop group using a number of well-known identities.[6]

For systems of fiber bundles with this structure a theorem has been proved regarding the circulation of the connectivity,[7] on the basis of which conditions are determined under which anomalies in the physical characteristics of films can be realized. Because the connection of a smooth fiber bundle of the space corresponds to a distortion 4-vector in the model used here, while the dislocation flux density tensor corresponds to components of a curvature 2-form, in accordance with the theorem on the transport of connections we should seek a realization of anomalies in the physical characteristics of the film using the condition

$$\alpha_{\mu\nu;\,\nu}=0. \qquad (1)$$

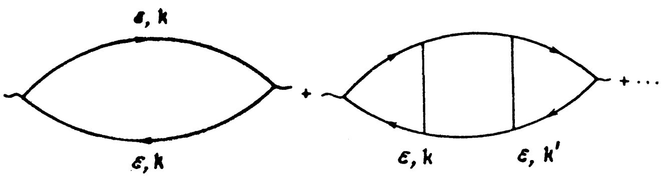
where $\alpha_{\mu\nu}$ is the dislocation flux density tensor.

The goal of this paper is to determine the character of quantum corrections to the conductivity of a polycrystalline thin film when condition (1) holds.

The conductivity $\sigma_{\mu\nu}$, according to the Kubo formula, can be written in the form:

$$\sigma_{\mu\nu}(\mathbf{q},\omega)=i\int_{-\infty}^{0} dt\langle[j_\mu(\mathbf{q},0),j_\nu(-\mathbf{q},t)]\rangle \times\frac{\exp(i\omega t)}{i\omega}-\frac{ne^2}{i\omega}\delta_{\mu\nu}, \qquad (2)$$

where j_μ is the current density, and n is the carrier concentration. The current correlator can be reduced to diagrams:



(3)

Here $\mathbf{q}=0$.

The contribution of the first diagram to the conductivity reduces to the expression

$$\sigma_{ij}=e^2\int d\varepsilon\,(2\pi\omega)^{-1}[f(\varepsilon-\hbar\omega)-f(\varepsilon)]\,d^2\mathbf{k}\,(2\pi)^{-2} \times\sum_\sigma v_i(\mathbf{k})v_j(\mathbf{k})G_\sigma^R(\varepsilon,\mathbf{k})G_\sigma^A(\varepsilon',\mathbf{k}),$$

where $v_i(\mathbf{k})$ is the ith component of the velocity; $\varepsilon'=\varepsilon-\hbar\omega$, and

$$G_\sigma^R=[\varepsilon+(i\hbar/2\tau-E_\mathbf{k})]^{-1},$$

$$G_\sigma^A=[\varepsilon-(i\hbar/2\tau-E_\mathbf{k})]^{-1}.$$

Here E_k is the kinetic energy, z is the dimensionality of the electron subsystem, and τ is the lifetime in a state with definite momentum.

After calculations based on the usual scheme, we obtain the following expression for the first term in the diagram:

$$\sigma_{ij}^{\mathrm{I}}=\delta_{ij}\frac{ne^2\tau/m}{1-i\omega\tau}, \qquad (5)$$

which for the case of isotropic scattering determines the principal contribution to the conductivity.

The second term in the diagrammatic series (3) reduces to the expression:

$$\sigma_{ij}^{\mathrm{II}}=e^2\int d\varepsilon\,\frac{f(\varepsilon-\hbar\omega)-f(\varepsilon)}{2\pi\varepsilon}\int\frac{d^2\mathbf{k}}{(2\pi)^2}\int\frac{d^2k'}{(2\pi)^2}\sum_{\sigma,\sigma'}v_i(\mathbf{k})\cdot \times v_j(\mathbf{k})G_\sigma^R(\varepsilon,\mathbf{k})G_\sigma^A(\varepsilon',\mathbf{k})\Gamma_{\sigma\sigma'}(\mathbf{k},\mathbf{k}',\varepsilon,\omega) \times G_{\sigma'}^R(\varepsilon,\mathbf{k}')G_{\sigma'}^A(\varepsilon',\mathbf{k}'), \qquad (6)$$

where the quantity $\Gamma_{\sigma\sigma'}$ is defined by the diagrammatic series

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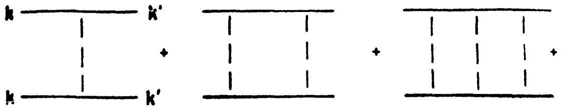


$$(7)$$

Here the dashed lines that separate the propagators represent scattering by defects and changes in quasimomentum.

For the second integral in (6) it is not difficult to obtain the expression

$$-2\pi i N(\varepsilon_F)\frac{2\hbar \mathbf{v}_F\mathbf{q}}{(\hbar\omega+i\hbar/\tau)\hbar\mathbf{v}_F\mathbf{q}[(\hbar\omega+i\hbar/\tau)^2-\hbar\mathbf{v}_F\mathbf{q}]}, \quad (8)$$

where $\mathbf{q}=\mathbf{K}+\mathbf{K}'$, and $N(\varepsilon_F)$ and v_F are the density of states and velocity at the Fermi level, respectively.

For small changes in the quasimomentum, Eq. (8) acquires the following form in the low-frequency limit:

$$\approx 4\pi N(\varepsilon_F)(\tau/\hbar)^3. \quad (9)$$

Then the conductivity tensor reduced to principal axes is

$$\sigma_{ij}=\sigma\delta_{ij}, \quad (10)$$

where

$$\sigma=\frac{2\pi N(\varepsilon_F)\tau}{\hbar}\frac{e^2}{\pi\hbar}z^{-1}v_F{}^2\tau^2\sum_{\sigma,\sigma'}\int\frac{d^2\mathbf{q}}{(2\pi)^2}\Gamma(\mathbf{q},\omega). \quad (11)$$

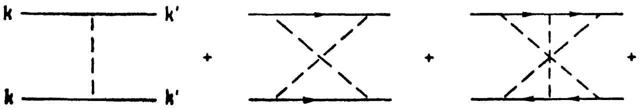
In order to calculate the quantity $\Gamma(q,\omega)$, we use the corresponding diagrammatic expansion

$$\sum_{\mathbf{q}_1,\mathbf{q}_2} V_{\mathbf{q}_1}G^R_{\mathbf{k}+\mathbf{q}_1}(\varepsilon)V_{\mathbf{q}_2}G^R_{\mathbf{k}+\mathbf{q}_1+\mathbf{q}_2}(\varepsilon)V_{\mathbf{q}_3}V^*_{\mathbf{q}_1}G^A_{\mathbf{k}'-\mathbf{q}_1}(\varepsilon')$$

$$\times V_{\mathbf{q}_2}{}^*G^A_{\mathbf{k}'-\mathbf{q}_1-\mathbf{q}_2}(\varepsilon')V_{\mathbf{q}_3}{}^*, \quad (12)$$

where v_{qi} are matrix elements.

Equation (12) corresponds to the third term of the diagrammatic series:



$$(13)$$

If we limit ourselves to isotropic scattering, then

$$|V_{\mathbf{q}_1}|^2=|V_{\mathbf{q}_2}|^2=[2\pi\tau N(\varepsilon_F)]^{-1}\hbar=\Gamma_0. \quad (14)$$

Introducing the notation

$$\Pi_{\mathbf{k}+\mathbf{k}'}(\varepsilon,\omega)=\sum_{\mathbf{q}}G^R_{\mathbf{k}+\mathbf{q}}(\varepsilon)G^A_{\mathbf{k}'-\mathbf{q}}(\varepsilon'), \quad (15)$$

the propagator we seek can be written as

$$\Gamma_0\Pi_{\mathbf{k}+\mathbf{k}'}\Gamma_0\Pi_{\mathbf{k}+\mathbf{k}'}\Gamma_0,$$

and the diagrammatic series can be written in the form

$$\Gamma=\Gamma_0+\Gamma_0\Pi\Gamma_0+\Gamma_0\Pi\Gamma_0\Pi\Gamma_0+\ldots=\frac{\Gamma_0}{i-\Gamma_0\Pi}. \quad (16)$$

This latter expression can be written in the form of a Dyson equation

$$\Gamma=\Gamma_0+\Gamma_0\Pi\Gamma.$$

An estimate of the quantity $\Pi_{\mathbf{k}+\mathbf{k}'}$ for small $|\mathbf{q}|$ leads to the following expression for Γ:

$$\Gamma_{\mathbf{k}+\mathbf{k}'}(\omega)=\frac{\hbar}{2\pi N(\varepsilon_F)\tau}[D(\mathbf{k}+\mathbf{k}')^2\tau-i\omega\tau]^{-1}, \quad (17)$$

where $D=z^{-1}v_F{}^2\tau$.

Then the conductivity is obtained in the form

$$\sigma(\omega)=-\frac{2e^2}{\pi\hbar}D\tau\int\frac{d^2q}{(2\pi)^2}(Dq^2\tau-i\omega\tau)^{-1}. \quad (18)$$

For thin films in the low frequency limit,

$$\sigma(0)=-\frac{e^2}{2\pi^2\hbar}\ln(\tau_i/\tau), \quad (19)$$

where τ_i is the relaxation time for inelastic scattering.

We now use the fact that the connectivity coefficients of the smooth fibration $P(R^4\oplus V^\infty, U(1))$ are the components of a distortion field. If $G_{r-r'}$ is the Green's function of the system without distortion, then in the presence of a distortion field β the corresponding Green's function has the form

$$\tilde{G}_{r-r'}=G_{r-r'}\exp\left[i\gamma\int_{r'}^{r}\beta(s)\,ds\right], \quad (20)$$

where γ is a coefficient that depends on the system of units chosen.

We note that in the model used here, because the structure group $U(1)$ is commutative, its structure constants equal zero; therefore the connection between the curvature tensor $R_{\mu\nu}$ and the connectivity coefficients Γ_μ of a fiber bundle of the space simplifies, and takes the form

$$R_{\mu\nu}=\partial_{[\mu}\Gamma_{\nu]}. \quad (21)$$

As for the physical meaning of the geometric characteristics in this model, Eq. (21) determines the generalized equation of the continuum theory of dislocations, i.e.[8]

$$\alpha_{\mu\nu}=\partial_{[\mu}\beta_{\nu]}, \quad (22)$$

where α is the dislocation flux density tensor, and β is a distortion 4-vector.

As a result of variation of the Lagrangian constructed here, taking into account the interaction of the fermion and distortion fields, we obtain a relativisitc equation of motion for the electron subsystem. Its nonrelativistic limit has the form

$$i\frac{\partial\Psi}{\partial t}=\left[-\frac{1}{2m}(\nabla^2-i\nabla\hat\beta-i\hat\beta\nabla+\hat\beta^2)+\hat\beta_0-\frac{\sigma}{2m}\hat\alpha\right]\Psi, \quad (23)$$

where $\hat\beta$ is the reduced 3-tensor of the distortion, $\hat\beta_0$ is the time component of the distortion 4-vector, $\hat\alpha$ is the dislocation flux density 3-tensor, and σ are Pauli matrices.

Now, using Eqs. (20) and (22), based on the formalism presented here we obtain for $\sigma^{\mathrm{II}}(\alpha)$

$$\sigma^{\mathrm{II}}(\alpha)=-\frac{2e^2}{\pi\hbar}D\tau\frac{\gamma\alpha}{\pi}\sum_{n=0}^{(D\tau\gamma\alpha)^{-1}}\left[4D\tau\gamma\alpha\left(n+\frac{1}{2}\right)+\frac{\tau}{\tau_i}\right], \quad (24)$$

where α is determined by the expression

$$\alpha_{ij}=\alpha\delta_{ij}. \quad (25)$$

Equation (24) is a quantum correction to the conductivity

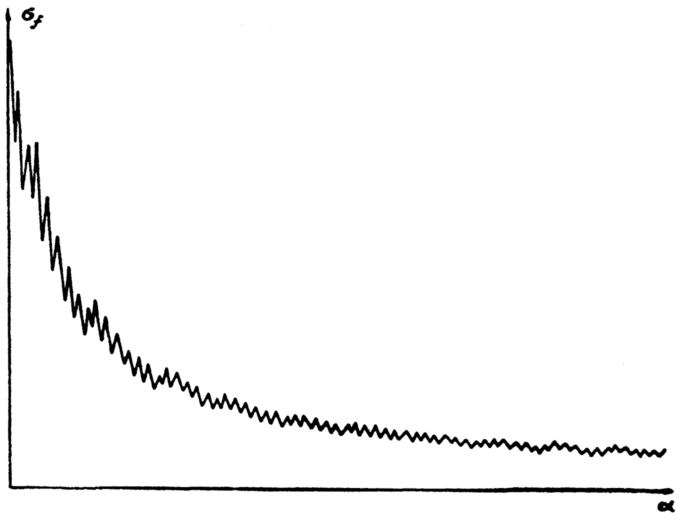


FIG. 1.

of a polycrystalline sample. The expression for the specific conductance of a thin film with thickness t has the form

$$\rho_f=\left\{\left[\frac{f[\chi(\alpha)]}{\rho_0}+\sigma^{II}(\alpha)\right]\left[1-\frac{A}{f[\chi(\alpha)]}\right]\right\}^{-1}, \quad (26)$$

where ρ_0 is the specific conductance of a bulk single crystal sample, and

$$f[\chi(\alpha)]=1-{}^3/_2\chi(\alpha)+3\chi^2(\alpha)-3\chi^3(\alpha)\ln[1+\chi^{-1}(\alpha)], \quad (27)$$

$$\chi(\alpha)=\frac{l_0}{d}\frac{1-D(\alpha)}{D(\alpha)}, \quad (28)$$

$$A=\frac{6}{\pi\lambda}(1-p)\int_0^{\pi/2}d\varphi\int_0^{\infty}dt'\,\frac{\cos^2\varphi}{H^2}\left[\frac{1}{t'^3}-\frac{1}{t'^5}\right]\frac{1-\exp(-\lambda t'H)}{1-p\exp(-\lambda t'H)}, \quad (29)$$

$$H(t',\varphi)=1-\chi(\alpha)\cos^{-1}\varphi\left[1-\frac{1}{t'^2}\right]^{-1/2}, \quad \lambda=\frac{t}{l_0}, \quad (30)$$

where d is the mean size of the grains; l_0 is the mean free path of a carrier in a bulk single crystal; $D(\alpha)$ is the probability density for passage of a carrier through a grain boundary.

Analysis of Eqs. (24) and (26)–(30) indicates the presence of quantum oscillations in the conductivity under the action of the distortion field. It is clear from Eq. (24) that the frequency and amplitude of the oscillations in the conductivity are determined by the intensity of the distortion. The function $\sigma_f(\alpha)$ is shown in Fig. 1.

Thus, in their geometric aspect these anomalies are a consequence of the theorem on the transport of the connection of the primary fibration of the space.

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