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Reciprocity relations for mechanically induced spin currents in metals in a nonlinear regime

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In the Markov relaxation and locally quasi-equilibrium distribution approximation, analogues of Onzager's relations for the response functions of the spin current in the nonlinear by intense mechanical and thermodynamic effects regime were obtained by the Kubo method.

Keywords: locally quasi-equilibrium distribution, spin Hamiltonian, spin current, nonlinearity, reciprocity, streintronics, spin caloritronics, Peltier spin effect, Zeebeck spin effect.

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Introduction

Spin caloritronics, which is currently being formed, may create prerequisites for combining actively developing spin caloritronics and straintronics into a new section of thermodynamics. Experiments [1,2] have shown that the application of deformation can change the direction of the heat flow generated by magnetothermoelectric effects. Currently, the spin dynamics of collectivized conduction electrons in spintronics systems is modeled by Rashba and Dresselhaus Hamiltonians describing the interaction of the orbital moment of the conduction electron with its spin moment.[3]. Estimates show that this interaction, as well as the exchange interaction within the framework of the RCCI model [4], can provide coherence of spin polarization at microscopic distances (of the order of $0.1\,\mu$m), but it is not sufficient for effective macroscopic (of the order of 1 mm) polarization spin currents in polycrystalline samples.

The possibility of efficient generation of spin polarization in polycrystalline ferromagnetic samples using torsion distortion, the axis of which is perpendicular to the charge current density vector, is shown in paper [5]. This approach creates prerequisites for controlling significant heat fluxes in massive samples, not just films, using the methods of straintronics. It is necessary to construct and verify the analytical functions of the response of spin current and heat flow to electrical, mechanical and thermodynamic effects and the reciprocity relations for them for the optimization of the design and operating modes of spin thermal transport systems. At the same time, high efficiency of the heat pump is achieved with high densities of heat flows and high intensities of mechanical and electrical influences. Therefore, it is necessary to obtain analogs of the classical Onsager relations in a substantially nonlinear mode in terms of impacts.

The response functions of nonlinear systems to inhomogeneous alternating electrical and mechanical impacts in the presence of unsteady spin currents and thermodynamic flows are constructed using the Kubo method and reciprocity relations for them are proved in work [6]. However, this conclusion is obtained based on the assumption of additivity of the effects. The analysis conducted in the work [5] showed that with mechanical control of spin current generation, electric current and mechanical distortion affect the system multiplicatively. This case, as well as the mechanically induced generation of spin currents in non-magnetic materials, and the spincaloric effects accompanying it, requires separate consideration.

1. Spin Hamiltonian of a conduction electron in a deformed metal

Consider a homogeneous and isotropic polycrystalline metal. Let there be N nodes in the crystallite, each of which contains the same ions with an effective charge $+Ze$. Such a lattice creates an electric field

$$\mathbf{E}(\mathbf{r}) = -\frac{eZ}{4\pi\varepsilon_0}\sum_{k=1}^{N}\frac{\mathbf{r}-\mathbf{r}_k}{|\mathbf{r}-\mathbf{r}_k|^3}.$$

The spin-orbital addition to the electron energy has the form [7]:

$$\hat{V} = \frac{\hbar e}{2m^2c^2}\left[\mathbf{E}(\mathbf{r})\times\hat{\mathbf{p}}\right]\hat{\mathbf{s}}. \qquad (1)$$

Here m — the mass of an electron with charge $-e$. The wave function of the collectivized conduction electron is written down in the form of the Vanier function [8]:

$$\psi(\mathbf{r}) = \frac{1}{\sqrt{N}}\sum_{n=1}^{N}\Psi(\mathbf{r}-\mathbf{R}_n)\exp(i\mathbf{k}\mathbf{R}_n),$$

where $\mathbf{R}_n$ is the translation vector, and construct the spin Hamiltonian for the perturbation (1)

$$\hat{H} = -\frac{\hbar^2 e^2 Z}{8\pi\varepsilon_0 m^2 c^2 N}\hat{s}_\alpha \exp(i\mathbf{k}(\mathbf{R}_n - \mathbf{R}_m)) \times \left\langle \Psi(\mathbf{r}+\mathbf{r}_k-\mathbf{R}_m)\middle|\frac{\hat{l}_\alpha}{r^3}\middle|\Psi(\mathbf{r}+\mathbf{r}_k-\mathbf{R}_n)\right\rangle. \quad (2)$$

In the nearest neighbor approximation, the mean on the right side (2) is different from zero only for $\mathbf{R}_n - \mathbf{r}_k = 0$ or $\mathbf{a}_\nu$ and $\mathbf{R}_m - \mathbf{r}_k = 0$ or $\mathbf{a}_\nu$, where $\mathbf{a}_\nu$ is the vector drawn to the nearest neighbor

$$\hat{H} = -\frac{\hbar^2 e^2 Z}{4\pi\varepsilon_0 m^2 c^2}\hat{s}_\alpha \left\{\cos(\mathbf{k}\mathbf{a}_\nu)\mathrm{Re}\left\langle \Psi_\nu^+\middle|\frac{\hat{l}_\alpha}{r^3}\middle|\Psi\right\rangle + \sin(\mathbf{k}\mathbf{a}_\nu)\mathrm{Im}\left\langle \Psi_\nu^-\middle|\frac{\hat{l}_\alpha}{r^3}\middle|\Psi\right\rangle\right\}.$$

Here $\Psi_\nu^{+}(\mathbf{r}) = \Psi(\mathbf{r}+\mathbf{a}_\nu) \pm \Psi(\mathbf{r}-\mathbf{a}_\nu)$, and implies summation by v over pairs of symmetrically located nearest neighbors. Assuming $\mathbf{k} = \mathbf{p}/\hbar$, where $\mathbf{p}$ — the quasi-pulse of the conduction electrons, we obtain in the first order of vanishing by $\mathbf{p}\,\mathbf{a}_\nu$:

$$\hat{H} = \mathbf{J}\hat{\mathbf{s}}, \quad (3)$$

$$\mathbf{J} = -\frac{\hbar e^2 Z}{4\pi\varepsilon_0 m^2 c^2}(\mathbf{p}\mathbf{a}_\nu)\mathrm{Im}\left\langle \Psi_\nu^-\middle|\frac{\hat{\mathbf{l}}}{r^3}\middle|\Psi\right\rangle. \quad (4)$$

In undeformed crystallite $\mathbf{J} = 0$. The wave function and the moment operator in (4) are transformed according to the law with inhomogeneous distortion $r'_\alpha = r_\alpha + u_\alpha(\mathbf{r})$

$$\hat{l}'_\alpha = -i\varepsilon_{\alpha\beta\gamma} r'_\beta \frac{\partial}{\partial r'_\gamma} = \hat{l}_\alpha - i\varepsilon_{\alpha\beta\gamma}\left(u_\beta \frac{\partial}{\partial r_\gamma} - r_\beta \frac{\partial u_\delta}{\partial r_\gamma}\frac{\partial}{\partial r_\delta}\right),$$

$$\Psi(\mathbf{r}') = \Psi(\mathbf{r}) + \frac{\partial \Psi}{\partial r_\alpha}\frac{\partial u_\alpha}{\partial r_\beta} r_\beta.$$

With torsion distortion in the sample along the axis $\mathbf{n}$ of the form $\boldsymbol{\Omega}(\mathbf{r}) = \mathbf{n}(\mathbf{r}\mathbf{n})\omega$, where ω — linear torsion, limiting the calculation to the first degrees of distortion the following is obtained

$$\hat{l}'_\alpha = \hat{l}_\alpha + \omega\varepsilon_{\alpha\beta\gamma} n_\beta n_\delta (r_\delta \hat{l}_\gamma + r_\gamma \hat{l}_\delta),$$

$$\Psi(\mathbf{r}') = \Psi(\mathbf{r}) + i\omega n_\beta n_\delta r_\delta \hat{l}_\beta \Psi(\mathbf{r}).$$

$$J_{\alpha'} = -\frac{\hbar e^2 Z\omega}{2\pi\varepsilon_0 m^2 c^2}\varepsilon_{\alpha'\beta'\gamma'} n_{\beta'} n_{\delta'} p_{\sigma'} a_{\nu\sigma'} \mathrm{Im}\left\langle \Psi_\nu^-\middle|\frac{r_{\gamma'}\hat{l}_{\delta'}}{r^3}\middle|\Psi\right\rangle. \quad (5)$$

Ratio (5) is written in the coordinate system associated with the axes of the crystallite. Let us introduce a laboratory coordinate system tied to the instruments that set the conduction current and measure the spin components. The components of vectors and tensors in the laboratory system will be denoted by non-hatched indices, and the components of vectors and tensors in the coordinate system associated with the crystal axes will be denoted by hatched indices.

The quasi-pulse vectors and torsion axes are transformed from the laboratory system to the system of crystal axes $p_{\sigma'} = p_{\sigma'\sigma} p_\sigma$, and the vector $\mathbf{J}$ is transformed from the system of crystal axes to the laboratory system $J_\alpha = p^{-1}_{\alpha\alpha'} J_{\alpha'}$, where $p_{\alpha'\alpha}$ is a unitary rotation matrix. This transformation is inserted in the equation (5) and the vector $\mathbf{J}$ is averaged in the macroscopic domain over random uniformly distributed orientations of crystallites

$$\bar{\mathbf{J}} = \omega K\left[\mathbf{n}\times[\mathbf{p}\times\mathbf{n}]\right]. \quad (6)$$

Accordingly, the averaged spin Hamiltonian (3) takes the form

$$\hat{H} = \omega K(p_\alpha - n_\alpha n_\beta p_\beta)\hat{s}_\alpha, \quad (7)$$

$$K = \frac{\hbar e^2 Z}{12\pi\varepsilon_0 m^2 c^2}\mathrm{Im}\left\langle \Psi_\nu^-\middle|\mathbf{a}_\nu \frac{\lfloor \mathbf{r}\times\hat{\mathbf{l}}\rfloor}{r^3}\middle|\right\rangle. \quad (8)$$

The value K depends only on the properties of the crystal, it can be calculated in the axes of symmetry of the crystal.

2. Reciprocity relations for nonlinear medium

The spin moment density operators $\hat{\mathbf{s}}(\mathbf{r},t)$ and the spin Hamiltonian $\hat{h}(\mathbf{r},t)$ are introduced so that in the interaction representation

$$\hat{\mathbf{s}}(t) = \int_V \hat{\mathbf{s}}(\mathbf{r},t)d^3r, \ \ \hat{H}(t) = \int_V \hat{h}(\mathbf{r},t)d^3r \ [9].$$

Following Kubo [10] the average components of the spin moment density are written down

$$s_\alpha(\mathbf{r},t) = \langle \hat{s}_\alpha(\mathbf{r},t)\rangle = \mathrm{Sp}(\hat{s}_\alpha(\mathbf{r},t)\hat{\rho}(t)). \quad (9)$$

Here $\hat{\rho}(t)$ is the density operator. Dynamics of the density operator and the observables in the interaction representation, taking into account the relation (7) is described by the Neumann equations

$$i\hbar\frac{\partial\hat{\rho}}{\partial t} = \int_V K\omega(\mathbf{r}',t)\big(n_\alpha(\mathbf{r}',t)n_\beta(\mathbf{r}',t)p_\beta(\mathbf{r}',t) - p_\alpha(\mathbf{r}',t)\big)[\hat{s}_\alpha(\mathbf{r}',t),\hat{\rho}(t)]d^3r + [\hat{H}_r,\hat{\rho}(t)],$$

$$i\hbar\frac{\partial\hat{s}_\alpha(\mathbf{r},t)}{\partial t} = [\hat{s}_\alpha(\mathbf{r},t),\hat{H}_0], \quad (10)$$

Here $\hat{H}_r$ is the relaxation Hamiltonian, $\hat{H}_0 = \int_V \hat{h}_0(\mathbf{r},t)d^3r$ is the real stationary undisturbed Hamiltonian.

A locally quasi-equilibrium distribution with the density operator [11] is set in the system when there are no external mechanical impacts:

$$\hat{\rho}^q(t) = \exp\left\{-\Phi(t) - \int_V \theta(\mathbf{r},t)\hat{h}_0(\mathbf{r},t)d^3r\right\},$$

$$\Phi(t) = \ln\mathrm{Sp}\exp\left\{-\int_V \theta(\mathbf{r},t)\hat{h}_0(\mathbf{r},t)d^3r\right\}. \quad (11)$$

Here $\Phi(t)$ is the Massieu–Planck functional, $\theta(\mathbf{r}, t) = 1/(kT(\mathbf{r}, t))$, k is the Boltzmann constant, $T(\mathbf{r}, t)$ is the local temperature.

Let us choose the eigenfunctions of the Hamiltonian $\hat{H}_0$ corresponding to the energy levels E_n as a basis. The solution of the second von Neumann equation (10) takes the form

$$\hat{s_\alpha}(\mathbf{r}, t) = \exp(i\hat{H}_0 t/\hbar)\hat{s_\alpha}(\mathbf{r}, 0)\exp(-i\hat{H}_0 t/\hbar t),$$

$$s_{\alpha nm}(\mathbf{r}, t - t') = \exp(-i\omega_{nm} t')s_{\alpha nm}(\mathbf{r}, t). \quad (12)$$

Here $\omega_{nm} = (E_n - E_m)/\hbar$. Accordingly, taking into account the hermiticity of the observables and the sign change of all spin components during time inversion

$$\hat{s_\alpha}(\mathbf{r}, -t) = -\hat{s}^*_\alpha(\mathbf{r}, t),$$

$$s_{\alpha km}(\mathbf{r}, -t) = -s^*_{\alpha km}(t, \mathbf{r}) = -s_{\alpha mk}(\mathbf{r}, t). \quad (13)$$

Denote $\mathbf{f}(\mathbf{r}, t) = \omega(\mathbf{r}, t)\big[\mathbf{n}(\mathbf{r}, t)\times[\mathbf{p}(\mathbf{r}, t)\times\mathbf{n}(\mathbf{r}, t)]\big]$ — the vector of impact on the system. Since $\mathbf{p}(-t) = -\mathbf{p}(t)$, $\mathbf{n}(-t) = -\mathbf{n}(t)$, $\omega(-t) = \omega(t)$, then $\mathbf{f}(\mathbf{r}, -t) = -\mathbf{f}(\mathbf{r}, t)$. The following is obtained from the first equations (10) and (13)

$$\hat{\rho}(-t, \mathbf{f}(\mathbf{r}, -t)) = \hat{\rho}^*(t, -\mathbf{f}(\mathbf{r}, t)),$$

$$\rho_{nm}(-t, \mathbf{f}(\mathbf{r}, -t)) = \hat{\rho}^*_{nm}(t, -\mathbf{f}(\mathbf{r}, t)) = \rho_{mn}(t, -\mathbf{f}(\mathbf{r}, t)). \quad (14)$$

The first equation (10) in the Markov relaxation approximation in matrix form has the form

$$\frac{\partial \rho_{nm}(t, \mathbf{f}, T)}{\partial t} = \frac{\rho^q_{nm} - \rho_{nm}(t, \mathbf{f}, T)}{\tau_{nm}} - \frac{i}{\hbar}\int\limits_V f_\beta(\mathbf{r}, t)$$

$$\times \big(\rho_{nk}(t, \mathbf{f}, T)s_{\beta km}(\mathbf{r}, t) - s_{\beta nk}(\mathbf{r}, t)\rho_{km}(t, \mathbf{f}, T)\big)d^3r. \quad (15)$$

Here $\tau_{nm} = \tau_{mn}$ — real positive relaxation times, and it is assumed that at time t_0 the system was in a quasi-equilibrium state with the density operator $\hat{\rho}^0$. Here and further, the dependence of $\mathbf{f}$ and T on time and coordinates is implied. We will look for a solution to equation (15) in the form $\rho_{nm}(t, \mathbf{f}, T) = \tilde{\rho}_{nm}(\mathbf{f}, T)\exp(i\omega_{nm} t)$. Taking into account the second equation (14), we obtain

$$\tilde{\rho}_{nm}\big(\mathbf{f}(\mathbf{r}, t), T(\mathbf{r}, t)\big) = \tilde{\rho}_{mn}\big(-\mathbf{f}(\mathbf{r}, t), T(\mathbf{r}, t)\big) \quad (16)$$

with simultaneous replacement of all frequencies ω_{nm} with ω_{mn}.

Equation (15) is equivalent to integral equation

$$\rho_{nm}(t) = (\rho^0_{nm} + \rho^q_{nm}(t))\exp\left(\frac{t_0 - t}{\tau_{nm}}\right) - \rho^q_{nm}(t)$$

$$+ \int\limits_{t_0}^{t}\exp\left(\frac{t' - t}{\tau_{nm}}\right)\frac{d\rho^q_{nm}(t')}{dt'}dt' + \frac{i}{\hbar}\int\limits_V\int\limits_{t_0}^{t}\exp\left(\frac{t' - t}{\tau_{nm}}\right)$$

$$\times f_\beta(\mathbf{r}', t')\Big(s_{\beta nl}(\mathbf{r}', t')\rho_{lm}(t') - \rho_{nl}(t')s_{\beta lm}(\mathbf{r}', t')\Big)dt'd^3r'. \quad (17)$$

Integration is performed in parts here in the integral containing ρ^q_{nm}. In relation (16) and further, the argument of functions of the form $\mathbf{f}(\mathbf{r}, t)$ implies that the functions depend on the values of the arguments at all times preceding t, and in the entire domain V.

It is possible to introduce a flux density operator satisfying the continuity equation $\hat{h}_0(\mathbf{r}, t)/\partial t = -\partial\hat{q}_{0\alpha}(\mathbf{r}, t)/\partial r_\alpha$, $\alpha = 1, 2, 3$ for a quasi-local density operator of an undisturbed Hamiltonian [9]. Then according to the equation (11)

$$\frac{d\hat{\rho}^q(t)}{dt} = -\hat{\rho}^q\int\limits_V\left\{\frac{\partial\theta(\mathbf{r}, t)}{\partial t}\hat{h}_0(\mathbf{r}, t) + \hat{q}_{0\alpha}(\mathbf{r}, t)\frac{\partial\theta(\mathbf{r}, t)}{\partial r_\alpha}\right\}d^3r$$

$$+ \hat{\rho}^q(t)\theta_k(t)Q_k(t) - \hat{\rho}^q(t)\frac{d\Phi}{dt}. \quad (18)$$

Here $\hat{Q}_k(t) = \int\limits_{S_k} n_{k\alpha}(\mathbf{r})\hat{q}_{0\alpha}(\mathbf{r}, t)d^2r$ —operators of energy flows through k-th contact, $\theta_k(t) = \theta(t, \mathbf{r}_k)$, $\mathbf{r}_k$ — coordinate of the center of k-th contact, $n_{k\alpha}$ — α-projection of the external normal to the surface of the k-th contact. Along with spin observables $\hat{s_\alpha}(\mathbf{r})$ and their corresponding mechanical impact $f_\alpha(\mathbf{r}, t)$, it is possible to introduce thermodynamic observables — energy density $\hat{h}_0(\mathbf{r})$, projections of energy flux densities $\hat{q}_{0\alpha}(\mathbf{r}, t)$, energy flows through kth contact — $\hat{Q}_k(t)$ and their corresponding thermodynamic effects $\partial\theta/\partial t$, $\partial\theta/\partial r_\alpha$, $\theta_k(t)$. The thermodynamic observables will be denoted as Θ_α, and the corresponding thermodynamic effects as will be denoted as T_α.

Let moment of time t_0 in the formula (17) tend to $-\infty$, then the first term in the right-hand part is zero. Let us introduce a new variable $\tau = t - t'$. Taking into account the formula (18), the equation (17) takes the form

$$\rho_{nm}(t) = -\rho^q_{nm}(t) - \int\limits_0^\infty\exp\left(\frac{-\tau}{\tau_{nm}}\right)\rho^q_{nm}(t - \tau)\frac{d\Phi(t - \tau)}{dt}d\tau$$

$$- \frac{1}{2}\int\limits_V\int\limits_0^\infty\exp\left(\frac{-\tau}{\tau_{nm}}\right)\big(\Theta_{\beta nl}(t - \tau, \mathbf{r}')\rho^q_{lm}(t - \tau)$$

$$+ \rho^q_{nl}(t - \tau) + \Theta_{\beta lm}(\mathbf{r}', t - \tau)\big)T_\beta(\mathbf{r}', t - \tau)d\tau d^3r'$$

$$+ \frac{i}{\hbar}\int\limits_V\int\limits_0^\infty\exp\left(\frac{-\tau}{\tau_{nm}}\right)\big(s_{\beta nl}(\mathbf{r}', t - \tau)\rho_{lm}(t - \tau)$$

$$- \rho_{nl}(t - \tau)s_{\beta lm}(\mathbf{r}', t')\big)f_\beta(\mathbf{r}', t - \tau)d\tau d^3r'. \quad (19)$$

For the reaction of the average value of spin observables to mechanical action from the formula (19) we obtain

$$s_\alpha(\mathbf{r}, t, \mathbf{f}, \mathbf{T}) = \rho_{nm}(t, \mathbf{f}, \mathbf{T})s_{\alpha mn}(\mathbf{r}, t, \mathbf{f}, \mathbf{T}) = s^q_\alpha(\mathbf{r}, t)$$

$$+ \int\limits_V\int\limits_0^\infty\chi_{\alpha\beta}\mathbf{r}, \mathbf{r}', \tau, \mathbf{f}, \mathbf{T})f_\beta(\mathbf{r}', t - \tau)d\tau d^3r'. \quad (20)$$

Here the thermodynamic impacts are combined into a vector $\mathbf{T}(\mathbf{r}, t)$, the first term in the right part (20) has the form

$$s^q_\alpha(\mathbf{r}, t) = -\rho^q_{nm}(t) s_{imn}(\mathbf{r}, t) - \int\limits_0^\infty \exp\left(\frac{-\tau}{\tau_{nm}}\right)\rho^q_{nm}(t-\tau)$$

$$\times s_{imn}(\mathbf{r}, t)\,\frac{d\Phi(t-\tau)}{dt}\,d\tau \qquad (21)$$

and describes a quasi-equilibrium, i.e., in the absence of mechanical and thermodynamic effects, the value of the observed. The second term in (20) describes the response of the system to mechanical influences. The response functions of the system have the form of the Kubo formula [10]

$$\chi_{\alpha\beta}(\mathbf{r}, \mathbf{r}', \tau, \mathbf{f}, \mathbf{T}) = \frac{iK\rho_{nm}(\mathbf{f}, \mathbf{T})}{\hbar\exp(\tau/\tau_{nm})}$$

$$\times \left\{\hat{s}_\alpha(\mathbf{r}, t)\hat{s}_\beta(\mathbf{r}', t-\tau) - \hat{s}_\beta(\mathbf{r}', t-\tau)\hat{s}_\alpha(\mathbf{r}, t)\right\}_{mn}.$$

We transform this formula taking into account the second equation (12) for $t' = t - \tau/2$

$$\chi_{\alpha\beta}(\mathbf{r}, \mathbf{r}', \tau, \mathbf{f}, \mathbf{T}) = \frac{iK\tilde{\rho}_{nm}(\mathbf{f}, \mathbf{T})}{\hbar\exp(\tau/\tau_{nm})}\exp\left(i\omega_{nm}\frac{\tau}{2}\right)$$

$$\times \left\{s_{\alpha ml}\left(\mathbf{r}, \frac{\tau}{2}\right)s_{\beta ln}\left(\mathbf{r}', -\frac{\tau}{2}\right) - s_{\beta ml}\left(\mathbf{r}', -\frac{\tau}{2}\right)s_{\alpha ln}\left(\mathbf{r}, \frac{\tau}{2}\right)\right\}. \qquad (22)$$

The following is obtained taking into account the relations (19) and (22) from the formula (23)

$$\chi_{\beta\alpha}(\mathbf{r}, \mathbf{r}', \tau, -\mathbf{f}, \mathbf{T}) = \frac{iK\tilde{\rho}_{mn}(\mathbf{f}, \mathbf{T})}{\hbar\exp(\tau/\tau_{nm})}\exp\left(\frac{i\omega_{nm}\tau}{2}\right)$$

$$\times \left\{s_{\beta ml}\left(\mathbf{r}, \frac{\tau}{2}\right)s_{\alpha ln}\left(\mathbf{r}', -\frac{\tau}{2}\right) - s_{\alpha ml}\left(\mathbf{r}', -\frac{\tau}{2}\right)s_{\beta ln}\left(\mathbf{r}, \frac{\tau}{2}\right)\right\}.$$

Let us replace the indices $n \leftrightarrow m$ taking into account the ratios (16) and the symmetry of the matrix τ_{nm}:

$$\chi_{\beta\alpha}(\mathbf{r}, \mathbf{r}', \tau, -\mathbf{f}, \mathbf{T}) = \frac{iK\tilde{\rho}_{nm}(\mathbf{f}, \mathbf{T})}{\hbar\exp(\tau/\tau_{nm})}\exp\left(\frac{i\omega_{mn}\tau}{2}\right)$$

$$\times \left\{s_{\beta ln}\left(\mathbf{r}, -\frac{\tau}{2}\right)s_{\alpha ml}\left(\mathbf{r}', \frac{\tau}{2}\right) - s_{\alpha ln}\left(\mathbf{r}', \frac{\tau}{2}\right)s_{\beta ml}\left(\mathbf{r}, -\frac{\tau}{2}\right)\right\}. \qquad (23)$$

From comparing the formulas (22) with (23), we obtain reciprocity relations for the spin polarization response functions to the combined effect of torsion distortion and charge current

$$\chi_{\alpha\beta}\big(\mathbf{r}, \mathbf{r}', \tau, \mathbf{f}(\mathbf{r}, t), \mathbf{T}(\mathbf{r}, t)\big) = \chi_{\beta\alpha}\big(\mathbf{r}', \mathbf{r}, \tau, -\mathbf{f}(\mathbf{r}, t), \mathbf{T}(\mathbf{r}, t)\big). \qquad (24)$$

The nonlinearity of the system is manifested in the dependence of the response functions (22) and (23) on the impact. It is due to the fact that the averaging is carried out not according to the quasi-equilibrium density operator (11), but according to the current (19), which deviates from the quasi-equilibrium under intense influences. Such a deviation can be neglected and averaged over a quasi-equilibrium density operator for weak impacts. Then the right parts of the formulas (22) and (23) do not depend on the effect of **f**, i.e., the system will be linear. Assuming in (24)$\mathbf{f} = -\mathbf{f} = 0$, we obtain the classical Onsager symmetry relation.

Considering mechanically induced spin currents only in metals, we will use the approximation of an ideal fermi gas for conduction electrons. The applicability of this model is justified by the fact that the thermodynamics of a fermi system is determined by its microscopic structure only near the Fermi surface [12]. Experimental studies of the temperature dependence of the electron heat capacity in metals show that it corresponds well to the model of an ideal fermi gas. At the same time, for most metals, the effective mass of the conduction electron is close to the mass of the free electron. Therefore, in the ratios (4)–(7) and in determining the vector of mechanical action **f**, we can put $\mathbf{p} = -m\mathbf{j}/(en_e)$, where $\mathbf{j}$ — the charge current density, n_e — concentration of conduction electrons.

The spin current density tensor is associated with spin polarization

$$S_{\alpha\beta}(\mathbf{r}, t) = -s_\alpha(\mathbf{r}, t)j_\beta(\mathbf{r}, t)/(en_e). \qquad (25)$$

Let us consider the reaction of the spin current density tensor only to the combined effect of torsion distortion and charge current, and for simplicity we will assume that the direction of the torsion axis is constant in time and space. Then, taking into account the ratio (20), the formula (25) can be written as

$$S_{\alpha\beta}(\mathbf{r}, t, \omega\mathbf{f}, \mathbf{T}) = S^q_{\alpha\beta}(\mathbf{r}, t) + \int\limits_V\int\limits_0^\infty \chi_{\alpha\beta\gamma}(\mathbf{r}, \mathbf{r}', \tau, \omega\mathbf{j}, \mathbf{T}, t)$$

$$\times \omega(\mathbf{r}', t-\tau)\big(j_\gamma(\mathbf{r}', t-\tau) - n_\gamma n_\delta j_\delta(\mathbf{r}', t-\tau)\big)d\tau\, d^3r'. \qquad (26)$$

Here $S^q_{\alpha\beta}(\mathbf{r}, t)$ is a quasi-equilibrium spin current density tensor, and according to formulas (22) and (25):

$$\chi_{\alpha\beta\gamma}(\mathbf{r}, \mathbf{r}', \tau, \omega\mathbf{j}, \mathbf{T}, t) = \frac{iK_1\tilde{\rho}_{nm}(\omega\mathbf{j}, \mathbf{T})}{\hbar\exp(\tau/\tau_{nm})en_e}$$

$$\times \exp\left(i\omega_{mn}\frac{\tau}{2}\right)j_\beta(\mathbf{r}, t)\left\{s_{\alpha ml}\left(\mathbf{r}, \frac{\tau}{2}\right)s_{\gamma ln}\left(\mathbf{r}', -\frac{\tau}{2}\right)\right.$$

$$\left. - s_{\gamma ml}\left(\mathbf{r}', -\frac{\tau}{2}\right)s_{\alpha ln}\left(\mathbf{r}, \frac{\tau}{2}\right)\right\}$$

— the response function of the spin current density tensor to mechanical influences, $K_1 = -mK/(en_e)$. If the charge current distribution is homogeneous, then, by analogy with the derivation of the formula (24), we obtain the symmetry ratio for the response function of the spin current density tensor to mechanical impacts:

$$\chi_{\alpha\beta\gamma}(\mathbf{r}, \mathbf{r}', \tau, \omega\mathbf{j}, \mathbf{T}, t) = -\chi_{\gamma\beta\alpha}(\mathbf{r}', \mathbf{r}, \tau, -\omega\mathbf{j}, \mathbf{T}, t). \qquad (27)$$

3. Reciprocity of spinstrain caloric effects

The continuity equations for the density operators of the spin Hamiltonian and the spin component have the form

$$\hat{h}(\mathbf{r},t)/\partial t = -\partial\hat{q}_{s\beta}(\mathbf{r},t)/\partial r_\beta,$$

$$\hat{s}_\alpha(\mathbf{r},t)/\partial t = -\partial\hat{S}_{\alpha\beta}(\mathbf{r},t)/\partial r_\beta. \quad (28)$$

Here $\hat{q}_{s\beta}(\mathbf{r},t)$ is the spin energy flux density operator, $\hat{S}_{\alpha\beta}(\mathbf{r},t)$ is the spin current tensor density operator. Assuming in (25) the charge current density is a given function of time and coordinates, and not a dynamic variable, we assume

$$\hat{S}_{\alpha\beta}(\mathbf{r},t) = \hat{s}_\alpha(\mathbf{r},t)j_\beta(\mathbf{r},t)/(en_e). \quad (29)$$

Assuming taking into account the formula (5), $\hat{h}(\mathbf{r},t) = \hat{s}_\alpha(\mathbf{r},t)f_\alpha(\mathbf{r},t)$ and considering the mechanical action $\mathbf{f}(\mathbf{r},t)$ as a slowly changing function of time and coordinates, we obtain from the equations (28), (29) and (20):

$$\hat{q}_{s\gamma}(\mathbf{r},t) = K_1\hat{S}_{\alpha\gamma}(\mathbf{r},t)f_\alpha(\mathbf{r},t)$$

$$= K_1\hat{s}_\alpha(\mathbf{r},t)f_\alpha(\mathbf{r},t)j_\gamma(\mathbf{r},t)/(en_e). \quad (30)$$

The formula (30) describes the Peltier spin effect [13] — mechanically induced spin current creates a heat flow by analogy with the effect for a charge current. Accordingly

$$\hat{q}_{s\gamma}(\mathbf{r},t) = \frac{f_\alpha(\mathbf{r},t)j_\gamma(\mathbf{r},t)}{en_e} \times \int_V \int_0^\infty \chi_{\alpha\beta}(\mathbf{r},\mathbf{r}',\tau,\mathbf{f},\mathbf{T})f_\beta(\mathbf{r}',t-\tau)d\tau d^3r'.$$

The response function $\chi_{\alpha\beta}$ has the form (22) and satisfies the reciprocity relations (24). We introduce the system setting time τ_r and the relaxation distance r_r, such that all $\chi_{\alpha\beta}(|\mathbf{r}-\mathbf{r}'| > r_r, \tau > \tau_r) \equiv 0$ Then, if the function $\mathbf{f}(\mathbf{r},t)$ changes little at a distance of r_r and during τ_r, it is possible to enter a function of the response of the heat flux density to mechanical impact

$$\mathbf{q}_s(\mathbf{r},t) = \mathbf{j}(\mathbf{r},t)f_\alpha(\mathbf{r},t)f_\beta(\mathbf{r},t)\big(D_{\alpha\beta}(\mathbf{r},\mathbf{f},\mathbf{T}) + D_{\beta\alpha}(\mathbf{r},\mathbf{f},\mathbf{T})\big)/2, \quad (31)$$

and taking into account the ratio (24) to obtain reciprocity ratios for it

$$D_{\alpha\beta}(\mathbf{r},\mathbf{f},\mathbf{T}) = \frac{K_1}{en_e}\int_V\int_0^\infty \chi_{\alpha\beta}(\mathbf{r},\mathbf{r}',\tau,\mathbf{F},\mathbf{T})d\tau d^3r'$$

$$= D_{\beta\alpha}(\mathbf{r},-\mathbf{f},\mathbf{T}). \quad (32)$$

Let there be only one thermodynamic effect in the system — temperature gradient. Then, for an isotropic medium, the elements of the matrix (32) should have the form

$$D_{\alpha\beta}(\mathbf{r},\mathbf{f},\partial T/\partial\mathbf{r}) = D_{\alpha\beta}(\mathbf{r},|\mathbf{f}|,|\partial T/\partial\mathbf{r}|,\mathbf{f},\partial T/\partial\mathbf{r}).$$

From the second equality (32) it follows that

$$D_{\alpha\beta}(\mathbf{r},\mathbf{f},-\partial T/\partial\mathbf{r}) = D_{\alpha\beta}(\mathbf{r},-\mathbf{f},\partial T/\partial\mathbf{r}) = D_{\beta\alpha}(\mathbf{r},\mathbf{f},\partial T/\partial\mathbf{r}).$$

In turn, it follows from the relation (32) that the heat flux created by the spin current against the temperature gradient is equal to the flow created in the direction of the temperature gradient.

Conclusion

The effect that creates mechanically induced spin currents in the metal is understood as the coefficient before the spin operator in the spin Hamiltonian (7). For a deformed metal, this effect is expressed in terms of the charge current density and torsion distortion. The maximum spin polarization is achieved when the torsion axis is perpendicular to the charge current density vector $\mathbf{j}$. In this case, the average spin is oriented parallel or antiparallel, depending on the sign K, to the vector $\mathbf{j}$. The vectors of charge current density and torsion are multiplicatively included in the effect. This makes it possible to consider the mechanical stress as parametric and simulate the experimentally detected change in the direction of the heat flow generated by thermoelectric effects under the action of mechanical stresses [1,2]. The possibility of controlling heat flows using a spin current, described by equation (31), is experimentally confirmed in [14]. The proposed method for analysis of quantum transport effects resulting from polarization of the mechanically induced spin current forms the basis for design and optimization of parameters of efficient systems of heat transport.

Kinetic coefficients (22) were determined sensu Kubo [10] formally, without specifying the physical mechanism of this response and matrix elements. Such a definition is not intended for calculation and estimation of response functions, but for establishing their general properties, such as symmetry relations. Kinetic coefficients are calculated and estimated from the solution of kinetic equations. With this calculation, the requirements of the principle of symmetry of kinetic coefficients are satisfied automatically regardless of the relaxation mechanism, i.e., the type of a specific kinetic equation or matrix coefficients [15].

The classical Onsager symmetry relations of kinetic coefficients for linear systems were obtained based on the assumption that the average relaxation of spontaneous fluctuations in the system occurs in accordance with macroscopic laws. The Markov relaxation approximation corresponds to this assumption in the Kubo scheme [10] if the undisturbed Hamiltonian is stationary.

It is not yet possible to obtain reciprocity relations for nonlinear systems based on such general assumptions. In the proposed scheme, they should be supplemented with the condition that the undisturbed system is in a quasi-equilibrium state (11), and the system remains stable under the action of a perturbation, which can be represented as the sum of products of a classical given function by the operator of the corresponding external dynamic variable and the Markov relaxation operator to a quasi-equilibrium state. The applicability of the Markovian relaxation and the locally quasi-equilibrium operator was examined respectively in [16,17].

Since the charge current and torsion density vectors enter multiplicatively in the spin perturbation (8), the construction of response functions according to the Kubo scheme describing spin-strain caloric effects in a form that allows obtaining symmetry relations for them required additional assumptions about the system. Such assumptions are the representation of the wave function of a collectivized conduction electron in the form of a Vanier function and the approximation of the nearest neighbors in the Hamiltonian (2), as well as the model of an ideal Fermi gas for conduction electrons. The applicability of these models for a specific task should be justified experimentally. Reliable experimental data on the spin Hall effect in metals are currently available. Therefore, the coefficients of the spin Hall effect of non-magnetic metals of the 5th and 6th periods [18] were calculated using the described approximations. The results of the calculations are consistent with the experimental ones within the margin of error.

The proposed approach to the derivation of reciprocity relations in nonlinear systems allows substantiating fairly general conclusions, for example, about the independence of the heat flux generated by the spin current from the direction of the temperature gradient. This conclusion allows for a experimental verification in a wide range of impact intensities.

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Conflict of interest

The author declares that he has no conflict of interest.

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