

Piezo-magnetoelectric effects in *p*-doped semiconductors

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We predict the appearance of a uniform magnetization in strained three-dimensional *p*-doped semiconductors with inversion symmetry breaking subject to an external electric field. We compute the magnetization response to the electric field as a function of the direction and magnitude of the applied strain. This effect could be used to manipulate the collective magnetic moment of hole mediated ferromagnetism of magnetically doped semiconductors.

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Antiferromagnetic dielectrics with inversion asymmetry exhibit the magnetoelectric (ME) effect, a phenomenon in which a static electric field induces a uniform magnetization.^{1,2} Moreover, as pointed out by Levitov *et al.*,³ a kinematic magnetoelectric (kME) effect can also occur in ostensibly nonmagnetic *conductors*, with spin-orbit coupling, which lack a center of inversion symmetry. Unlike in dielectrics, in the case of conductors, the electric field induced magnetization density $M_i = \alpha_{ij} E_j$ is necessarily accompanied by dissipation. Since \mathbf{M} is odd under time reversal (T) and \mathbf{E} is even, α_{ij} must be proportional to the relaxation time, a quantity related to the entropy production, making the process dissipative. In addition, since \mathbf{M} is even under parity (P) while \mathbf{E} is odd, α_{ij} is zero for parity invariant systems. The kME effect also vanishes in the absence of spin-orbit interaction. In two-dimensional (2D) *n*-doped inversion layers with Rashba spin-orbit interaction, this effect has been predicted more than a decade ago,^{4,5} with recent renewed theoretical interest,⁶⁻¹⁰ but has been observed experimentally only very recently.^{11,12}

In the model used by Levitov *et al.*,³ the kME effect originates from an electron scattering by impurities whose potential lacks inversion symmetry. As such, the effect is extrinsic and actually *vanishes* in the clean limit.

In contrast, we present an analysis of hole-doped bulk semiconductor without inversion symmetry where the spin-orbit splitting of the *p*-band is intrinsic. It is rather hard to obtain sizable parity-breaking terms in three-dimensional systems, especially in the valence band. In the absence of strain the system is both T and P invariant and hence no kME effect occurs. As we argue below, the shear strain induces a P -breaking term in the Hamiltonian which is responsible for the effect.

There are several advantages to having a piezomagneto-electric effect in 3D *p*-doped semiconductors (such as GaAs, GaSb, InSb, InGaAs, and AlGaAs). Technologically, engineering of different original strain architectures is a common procedure in today's semiconductor applications. By taking place in a 3D bulk sample, rather than in a 2D sample, this effect allows (with specific strain configurations) full spatial manipulation of the magnetic moment. Most importantly, the effect occurs in *p*-doped semiconductors, and thus it allows manipulation of the direction of the collective ferromagnetic moment which develops in (*p*-doped) dilute magnetic semiconductors.

Within the spherical approximation,^{13,14} the effective Hamiltonian of a hole-doped semiconductor with spin-orbit coupling is described by the Luttinger-Kohn model in the spin-3/2 band

$$H_{LK} = \frac{1}{2m} \left(\gamma_1 + \frac{5}{2} \gamma_2 \right) \mathbf{k}^2 - \frac{1}{m} \gamma_2 (\mathbf{k} \cdot \mathbf{S})^2, \quad (1)$$

where S_i is the spin-3/2 (4×4 matrix) operator, γ_1 and γ_2 are material-dependent Luttinger constants. The band structure consists of a doubly degenerate heavy hole band corresponding to $\hat{\mathbf{k}} \cdot \mathbf{S} = \pm 3/2$ and a doubly degenerate light hole band with $\hat{\mathbf{k}} \cdot \mathbf{S} = \pm 1/2$ (see inset of Fig. 1). The above Hamiltonian is both P and T invariant. The strain, being a second order symmetric tensor ϵ_{ij} , naturally couples to $S_i S_j$

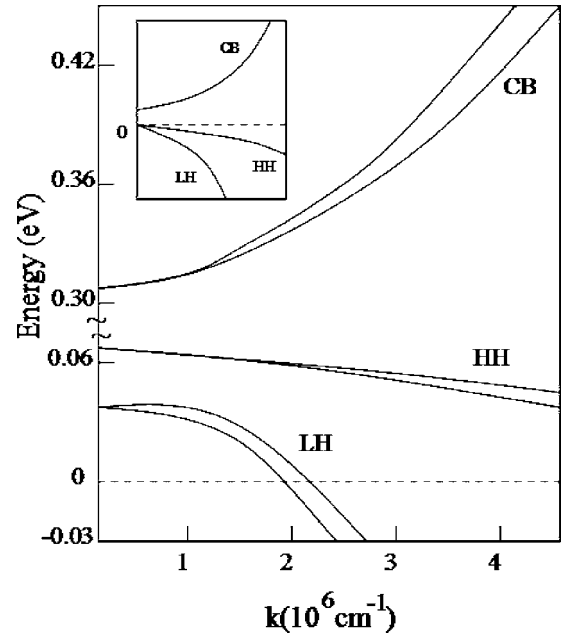


FIG. 1. Dispersion curves for InSb at 4 kbar stress on the [110] direction ($\epsilon_{xy} \approx 2 \times 10^{-3}$) and $\vec{k} \parallel [1\bar{1}0]$ as measured by Seiler *et al.* (Ref. 16). The strain splits the conduction and the valence bands. The Dresselhaus k^3 type inversion asymmetry is negligibly small on this scale. No splitting is observed for strain in the [001] direction.

and to zeroth order modifies the original Hamiltonian H_{LK} by the term

$$H_\epsilon = D_d(\epsilon_{xx} + \epsilon_{yy} + \epsilon_{zz}) + D_u\epsilon_{ij}S_iS_j, \quad i, j = x, y, z, \quad (2)$$

where D_d and D_u are the usual hydrostatic and shear deformation potentials.¹⁵ The modified Hamiltonian $H_{LK} + H_\epsilon$ remains invariant under both P and T . Each of the two valence bands is still doubly degenerate. As seen in Fig. 1, the strained Hamiltonian exhibits a finite energy gap between the heavy and light hole bands at zero momentum $\mathbf{k}=0$. External electric field will cause a spin current,¹³ but no uniform magnetization. For semiconductors with inversion symmetry these are the only terms allowed at quadratic order in \mathbf{k} .

However, in the absence of an inversion symmetry center, the shear strain induces a P -breaking term *linear* in momentum¹⁵

$$H' = \lambda_i S_i, \quad \lambda_x = C_4(\epsilon_{xy}k_y - \epsilon_{xz}k_z), \quad (3)$$

where λ_y, λ_z are obtained from λ_x by cyclic permutation of indices and C_4 is a material constant related to the interband-deformation potential for acoustic phonons. This term is responsible for the piezo-kME effect. Its origin can be traced back to the Kane's 8×8 model (2×2 for each the conduction and the split-off band, and 4×4 for the valence band) (Fig. 1), within which the valence band couples to both the conduction band and the split-off band. Upon straining, the zeroth order effect is the P -invariant coupling mentioned in the previous paragraph. At the first order, the conduction band $|s\rangle$ and the valence bands $|x\rangle, |y\rangle, |z\rangle$ couple, and the matrix elements between the valence and conduction band have the form $\epsilon_{xy}\langle s|\partial_x\partial_y|z\rangle$ (plus cyclic permutations) where $|s\rangle$ is the s orbital and $|z\rangle$ is one of the p orbitals. Any other combination will not satisfy the L_z selection rule. In systems with inversion symmetry where the selection rules for \mathbf{L} are satisfied, it is impossible to couple the spin-0 ($|s\rangle$) conduction states with spin-1 ($|x\rangle, |y\rangle, |z\rangle$) valence states through a spin-2 term (rank 2 tensor) (ϵ_{ij}) and hence $\langle s|\partial_x\partial_y|z\rangle=0$. However, when inversion symmetry is broken, $\langle s|\partial_x\partial_y|z\rangle \neq 0$ as the \mathbf{L} selection rule does not apply. We then obtain an 8×8 Kane matrix with the strain terms describing the interaction between valence and conduction bands. To find an effective 4×4 Hamiltonian for the valence band, one must project onto the valence band while taking into account the interactions with the conduction and the split-off band. The first term which appears in perturbation theory is the Hamiltonian (3). Reciprocally, a similar term will appear in the conduction band, with the spin there being a spin-1/2 matrix. These terms have been observed experimentally¹⁶ although recent evidence suggests other effects could also play a role.¹¹

The piezo-kME effect can be easily understood as follows: assume a material strained only along the $[110]$ direction, such that $\epsilon_{xy} \neq 0$ is the only nonvanishing shear strain component. Hence, the P -breaking term in the Hamiltonian is $H' = C_4(\epsilon_{xy}k_y S_x - \epsilon_{yx}k_x S_y)$. This effectively corresponds to Zeeman coupling of hole spins with a fictitious internal magnetic field $B_x = C_4\epsilon_{xy}k_y/\mu_B$, $B_y = -C_4\epsilon_{yx}k_x/\mu_B$, μ_B being the Bohr magneton. Upon the application of an electric

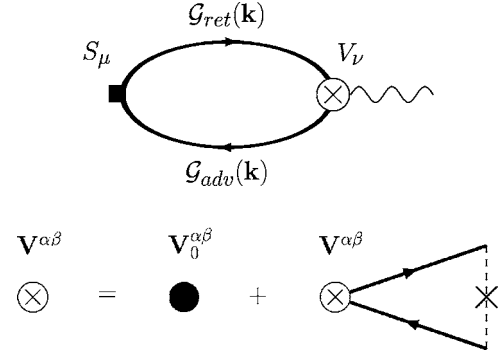


FIG. 2. Top: Feynman diagram representing the kinematic Magneto-Electric effect in 3D. Bottom: Kinetic equation for the vertex matrix in the ladder approximation. Here $V_0^{\alpha\beta}$ is the velocity operator in the absence of impurities.

field along, say, the y axis, the average momenta become $\langle k_x \rangle \approx 0$, $k_y \approx eE\tau/m$ where τ is the momentum relaxation time. In turn, this gives $\langle B_y \rangle \approx 0$, $\langle B_x \rangle \approx C_4\epsilon_{xy}eE\tau/m\mu_B$. The nonzero $\langle B_x \rangle$ field now couples to the spins and orients them along the x axis. This gives rise to a magnetization perpendicular to the electric field. Alternatively, the electric field along the x axis will induce magnetization along the y axis of equal modulus but of opposite sign to the previous one. This has recently been observed in the conduction band by Kato *et al.*¹¹ Moreover, if we assume linear dependence on the relaxation time τ and neglect the effect of parity conserving strain term, then the form of α_{ij} is constrained by dimensional analysis alone

$$\alpha_{ij} = \mu_B n^{2/3} \frac{e\tau}{\hbar} \times \Phi_{ij} \left(\frac{mC_4}{\gamma_1 \hbar^2 n^{1/3}}, \frac{\gamma_1}{\gamma_2} \right), \quad (4)$$

where n is the carrier density and the scaling function $\Phi_{ij}(x, y)$ vanishes linearly with its first argument x . Based on the above argument, up to a sign, its components should be proportional to ϵ_{ij} .

We shall now justify the above claims. The static spin response to the dc electric field can be shown to be given by

$$\alpha_{\mu\nu} = \frac{\mu_B}{\hbar} \lim_{\omega \rightarrow 0} \text{Im} \left[\frac{Q_{\mu\nu}^{\text{ret}}(\omega)}{\omega} \right], \quad (5)$$

where μ_B is the Bohr magneton and the retarded correlation function $Q_{\mu\nu}^{\text{ret}}(\omega) = Q_{\mu\nu}(i\omega \rightarrow \omega + i\eta)$, ($\eta \rightarrow 0^+$), and

$$Q_{\mu\nu}(i\omega) = \int_0^\beta d\tau e^{i\omega\tau} \langle TS_\mu(\tau)j_\nu(0) \rangle. \quad (6)$$

For dc response only spatial averages of the spin and the current operators need to be considered above. The corresponding diagram is shown in Fig. 2.

Since the strain splitting is typically small compared to the spin-orbit splitting at the Fermi surface (Fig. 1), we can include its effects within (degenerate) perturbation theory. Utilizing the powerful mapping between spin-3/2 $SU(2)$ and

SO(5) representations by Murakami, Nagaosa, and Zhang,¹³ the unperturbed thermal Green's functions can be conveniently written as

$$G_0(\mathbf{k}, i\omega_n) = \frac{1}{2} \sum_{s=\pm 1} \frac{1 + s\hat{d}_j(\mathbf{k})\Gamma_j}{-i\omega_n + (1 + s\Delta)\epsilon(\mathbf{k})}, \quad (7)$$

where $\Delta = 2\gamma_2/\gamma_1$, $\epsilon(\mathbf{k}) = \gamma_1 \mathbf{k}^2/2m$, $j = 1, \dots, 5$ and $\hat{d}(\mathbf{k})$ is a (spherical) unit vector in the five-dimensional space, equivalently $\hat{d}_m(\mathbf{k}) = Y_{l=2}^m(\theta_{\mathbf{k}}, \phi_{\mathbf{k}})$ where Y 's are spherical harmonics and the angles are in \mathbf{k} -space; Γ_j are five Dirac gamma matrices.¹³ Upon inclusion of spinless impurities with potential $u(\mathbf{k})$, the full (impurity) Green's function $G(\mathbf{k}, i\omega_n) = G_0[\mathbf{k}, i\omega_n + \Sigma(\mathbf{k}, i\omega_n)]$. Within the Born approximation the self-energy is $\Sigma(\mathbf{k}, i\omega_n) = n_{\text{imp}} \int d\mathbf{q} |u(\mathbf{k}-\mathbf{q})|^2 G_0(\mathbf{q}, i\omega_n)$; n_{imp} is the concentration of impurities. Finally, to leading order in P breaking strain¹⁷

$$\mathcal{G}(\mathbf{k}, i\omega_n) = [1 - G(\mathbf{k}, i\omega_n)H'(\mathbf{k})]G(\mathbf{k}, i\omega_n). \quad (8)$$

Subsequently, all of the calculations will be carried out using Eq. (8).

As shown in Fig. 2, the finite frequency response function (6) is given by

$$Q_{\mu\nu}(i\Omega) = -\frac{e}{\beta} \sum_{\omega_n} \int d\mathbf{k} \text{Tr}[S_{\mu}\Pi_{\nu}(\mathbf{k}, i\omega, i\Omega)], \quad (9)$$

where the trace is over the heavy/light hole spaces and where, as shown in Fig. 2, the (4×4) matrix vertex function Π_{ν} satisfies the kinetic equation (within the ladder approximation)

$$\begin{aligned} \Pi_{\mu}(\mathbf{k}, i\omega, i\Omega) &= \mathcal{G}(\mathbf{k}, i\omega)V_{\mu}(\mathbf{k})\mathcal{G}(\mathbf{k}, i\omega - i\Omega) \\ &+ n_{\text{imp}}\mathcal{G}(\mathbf{k}, i\omega) \int d\mathbf{q} |u(\mathbf{k}-\mathbf{q})|^2 \\ &\times \Pi_{\mu}(\mathbf{q}, i\omega, i\Omega)\mathcal{G}(\mathbf{k}, i\omega - i\Omega). \end{aligned} \quad (10)$$

The velocity operator $V_{\mu}(\mathbf{k}) = \partial H(\mathbf{k})/\partial k_{\mu}$. Note that \mathcal{G} does not commute with Π_{μ} . As such we have 16 coupled integral equations to solve, one for each entry of the 4×4 matrix. In the case of δ -function impurities $u(\mathbf{k}-\mathbf{q}) = u_0$ is a constant and the above integral equation is separable. Integrating both sides over \mathbf{k} , it is easy to see that in the absence of parity breaking strain, the vertex correction vanishes.¹⁸ On the other hand, for finite strain, the vertex correction does not vanish, and we still have to solve a system of 16 coupled equations.

However, to leading order in the strain it can be seen that *all 16 equations decouple in the basis of the Clifford algebra*. Expanding the vertex matrix

$$\Pi_{\mu}(\mathbf{k}, i\omega, i\Omega) = \sum_{A=0}^{15} \lambda_{\mu}^A(\mathbf{k}, i\omega, i\omega - i\Omega)\Gamma_A, \quad (11)$$

where the sum runs over all 16 elements¹⁹ and $\lambda_{\mu}^A(\mathbf{k}, i\omega, i\omega - i\Omega)$ is now an ordinary vector function. Since $\text{Tr}[\Gamma_A\Gamma_i\Gamma_B\Gamma_j]$ is diagonal in A and B it is easy to see that

$$\frac{1}{4} \int d\mathbf{k} \text{Tr}[\Gamma_A\mathcal{G}(\mathbf{k}, i\omega)\Gamma_B\mathcal{G}(\mathbf{k}, i\omega - i\Omega)] = M_A(i\omega, i\Omega)\delta_{AB}$$

Therefore,

$$\Pi_{\mu}(\mathbf{k}, i\omega, i\Omega) = \mathcal{G}(\mathbf{k}, i\omega)[V_{\mu}(\mathbf{k}) + R_{\mu}(i\omega, i\Omega)]\mathcal{G}(\mathbf{k}, i\omega - i\Omega). \quad (12)$$

where

$$R_{\mu}(i\omega, i\Omega) = n_{\text{imp}}u_0^2 \left(\sum_{A=0}^{15} \frac{\Gamma_A V_{\mu}^A(i\omega, i\Omega)}{1 - n_{\text{imp}}u_0^2 M_A(i\omega, i\Omega)} \right) \quad (13)$$

and

$$V_{\mu}^A(i\omega, i\Omega) = \frac{1}{4} \int d\mathbf{k} \text{Tr}[\Gamma_A\mathcal{G}(\mathbf{k}, i\omega)V_{\mu}(\mathbf{k})\mathcal{G}(\mathbf{k}, i\omega - i\Omega)], \quad (14)$$

$$M_A(i\omega, i\Omega) = \frac{1}{4} \int d\mathbf{k} \text{Tr}[\Gamma_A\mathcal{G}(\mathbf{k}, i\omega)\Gamma_A\mathcal{G}(\mathbf{k}, i\omega - i\Omega)]. \quad (15)$$

With the known structure of the vertex matrix (12), we can compute the response to the E_{μ} field. Following the standard technique²⁰ we can perform the Matsubara summation, let $i\Omega \rightarrow \Omega + i\eta$, take the limit of $\Omega \rightarrow 0$ and finally take the temperature $T \rightarrow 0$ to find

$$\alpha_{\mu\nu} = e \int d\mathbf{k} \text{Tr}[S_{\mu}\mathcal{G}^{\text{ret}}(\mathbf{k})[V_{\nu}(\mathbf{k}) + R_{\nu}]\mathcal{G}^{\text{adv}}(\mathbf{k})], \quad (16)$$

where the vertex matrix R_{μ} is given by the discontinuity of Eq. (13), $R_{\mu} = R_{\mu}(i\eta, -i\eta)$. Finally, ignoring the interband transitions, [i.e., in multiple sums over s in Eq. (7) we keep only the same s], we get

$$\alpha_{ij} = -\mu_B n^{1/3} \frac{\partial \lambda_i}{\partial k_j} \frac{e\tau}{\hbar^3} \frac{15}{2} \frac{3^{1/3}}{\pi^{1/3}} \frac{m}{\gamma_1} \left(\sum_{s=\pm 1} \frac{1}{(1+s\Delta)^{3/2}} \right)^{2/3}, \quad (17)$$

where τ is the momentum relaxation time, $\mu_B = 0.58 \times 10^{-8}$ eV/G is the Bohr magneton, n is the carrier concentration, and $\Delta = 2\gamma_2/\gamma_1$. Since $\lambda_x = C_4(\epsilon_{xy}k_y - \epsilon_{xz}k_z)$ (λ_y, λ_z being obtained through cyclic permutations of x, y, z) are linear in the components $k_{x,y,z}$, the factor $\partial \lambda_i / \partial k_j$ is a momentum independent, strain dependent tensor. For GaAs, $C_4 = C_3/2\eta$ where $C_3 = 8 \times 10^5$ m/s (Ref. 15) is a measured constant related to the deformation potential for acoustic phonons while $\eta = E_{SO}/(E_g + E_{SO}) = 0.183$, E_g being the gap energy while E_{SO} is the spin-orbit coupling energy for GaAs. For GaAs $\gamma_1 = 6.98$, $\gamma_2 = 2.06$, hence $\Delta = 0.59$. This gives a value of $C_4/\hbar = 2.2 \times 10^6$ m/s. For $n = 3 \times 10^{16}$ cm⁻³, $\epsilon_{xy} = 1\%$, in a generic sample of mobility $\mu = 50$ cm²/V \cdot s the magnetization due (and perpendicular) to an electric field E is $\langle S \rangle = 5 \times 10^{16}$ E(V⁻¹ m⁻²). Under an electric field of $E = 10^4$ V/m the magnetization becomes $\langle S \rangle = 6 \times 10^{14}$ cm⁻³. This corresponds to almost $\langle S \rangle/n = 2\%$ spin orientation efficiency. Since $\langle S \rangle \sim k_F \sim n^{1/3}$ the spin orientation efficiency will grow for decreasing hole concentration n . We now turn

to the question of validity of our approximations. The energy difference at the Fermi wave vector between the LH and HH bands is around 0.1 eV. This is larger by almost an order of magnitude than the splitting of the LH (or HH) bands due to strain, which is of the order $2C_4\epsilon k_F \sim 1.4 \times 10^{-2}$ eV, assuming a strain of 1%–2% and a density of roughly 10^{17} cm $^{-3}$. Hence, ignoring the interband transitions is expected to be a very good approximation. We also make two other approximations: first, we neglect the thermal fluctuations, by giving only the zero-temperature result, and second, we assume that the Dresselhaus-type term cubic in \mathbf{k} (which is present even in the absence of strain in inversion-asymmetric semiconductors) is small compared to the strain-induced linear term in \mathbf{k} . These conditions are $2C_4\epsilon k_F > kT$ and $2C_4\epsilon k_F > 2\alpha_v \hbar^3 k_F^3 / \sqrt{2m_e E_g}$, where α_v is a material constant ($\alpha_v = 0.027$ for GaAs) and m_e is the conduction band mass. For $T \approx 100$ K (the transition temperature of most magnetically doped semiconductors) and $\epsilon \sim 1\%$ – 2% , we find that our theoretical predictions are valid for a rather wide range of doping concentration 3×10^{16} cm $^{-3} < n < 10^{20}$ cm $^{-3}$.

An interesting new application of the piezo-kME effect would be to manipulate the collective magnetization of the dilute magnetic semiconductors.²¹ It is believed, at least in the high mobility metallic regime, that the ferromagnetism of Mn $^{++}$ ions in GaMnAs is hole mediated. Within the $\mathbf{k} \cdot \mathbf{p}$ method,^{22,23} the coupling between the collective magnetization and the electric field induced spin polarization is of

the order $Jn \approx 1 \mu\text{eV}$ for $n = 10^{16}$ cm $^{-3}$ and $Jn \approx 1$ meV for $n = 10^{19}$ cm $^{-3}$.^{22,23} While the effective field acting on the itinerant carrier is of the order of tens of tesla ($g\mu_B B_{\text{eff}} \sim C_4\epsilon k_F \approx 10$ meV) the field acting on the magnetic impurities is much lower due to the low value of the coupling constant. However, since our effect scales as $n^{1/3}$ it dominates the magnetic field produced by the electric current at low density. Also, near the second order magnetic transition, the effect of the carrier magnetization is magnified due to diverging susceptibility. The proposed experiment is as follows: above the Curie temperature, drive an electric current through the semiconductor. As per the effect proposed, the material will acquire a bulk uniform magnetization. Then cool down the system below the Curie temperature, such that it acquires a collective magnetization from the magnetic dopants. This magnetization should align (up to some stiffness due to a potential easy axis) with the uniform magnetization induced by the electric current. Repeat the experiment having the electric current switch sign. The collective magnetization should also switch sign.

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