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Spontaneous violation of reflectional symmetry in solids

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A model is suggested in which the reflectional symmetry of the electron Fermi liquid in metals or semiconductors is spontaneously violated. The properties of the asymmetric phase and the possibility of its experimental detection are discussed.

Reflectional symmetry imposes certain restrictions on the possible form of physical laws. It requires, for example, that in all vector relations like $\vec{A} = \vec{B}$, \vec{A} and $\overline{\mathbf{B}}$ should be both polar or both axial vectors. As we know, reflectional symmetry is violated in weak interactions. However, at ordinary energies this violation is very weak and is totally negligible on a macroscopic level. It has been recently suggested¹ that reflectional symmetry can be violated spontaneously as a result of a spin-dependent effective interaction of electrons in metals. Using Fermi-liquid theory, the authors have shown that if the interaction is strong enough, it may become energetically favorable for electrons to develop a nonzero average helicity, $\langle \vec{\sigma} \cdot \vec{k} \rangle \neq 0$. In the present paper we suggest a simple microscopic model with spontaneous violation of reflectional symmetry and discuss the physical properties of the asymmetric phase.

Our model is described by the Hamiltonian

$$H = \sum \epsilon_k a_{k\alpha}^{\dagger} a_{k\alpha} + U \quad , \tag{1}$$

where

$$U = -\frac{1}{2}g \sum_{k,k'} (\hat{k} \cdot \hat{k}') (\vec{\sigma}_{\alpha\beta} \cdot \vec{\sigma}_{\alpha'\beta'}) a^{\dagger}_{k\alpha} a^{\dagger}_{k'\alpha'} a_{k'\beta'} a_{k\beta} , \qquad (2)$$

 $\hat{k} = \vec{k}/k$, $k = |\vec{k}|$, $\sigma_{\alpha\beta}^{i}$ are the Pauli matrices, and g > 0. Here, and below, we assume summation over repeated spinor and vector indices. The electron-electron scattering amplitude is proportional to $(\hat{k} \cdot \hat{k}')(\vec{\sigma} \cdot \vec{\sigma}')$, and we have included only terms corresponding to the forward scattering (i.e., scattering does not change the momenta of the electrons, but can change their spins). The interaction (2) is to be understood as an effective interaction between quasiparticles, its spin dependence being attributable to exchange forces between electrons.²

In the Hartree-Fock approximation, the average interaction energy of the system equals

$$U = -\frac{1}{2}g \sum_{\boldsymbol{k},\boldsymbol{k}'} (\hat{\boldsymbol{k}} \cdot \hat{\boldsymbol{k}}') (\boldsymbol{\Sigma}_{\boldsymbol{k}} \cdot \boldsymbol{\Sigma}_{\boldsymbol{k}'}) \quad , \tag{3}$$

where

$$\vec{\Sigma}_{k} = \vec{\sigma}_{\alpha\beta} \langle a_{k\alpha}^{\dagger} a_{k\beta} \rangle \tag{4}$$

and the angular brackets mean quantum statistical averaging. The quantity $\langle a_{k\alpha}^{\dagger}a_{k\beta}\rangle$ can be represented as

$$\langle a_{k\alpha}^{\dagger} a_{k\beta} \rangle = \frac{1}{2} (\delta_{\beta\alpha} + \vec{\sigma}_{\beta\alpha} \cdot \hat{k}) n_{k+} + \frac{1}{2} (\delta_{\beta\alpha} - \vec{\sigma}_{\beta\alpha} \cdot \hat{k}) n_{k-} ,$$
 (5)

where n_{k+} and n_{k-} are the occupation numbers of states having definite helicity, $\sigma \equiv (\vec{\sigma} \cdot \hat{k}) = \pm 1$. Then we obtain

$$\vec{\Sigma}_{k} = \hat{k} (n_{k+} - n_{k-}) , \qquad (6)$$

$$\langle H \rangle = \sum_{k} \epsilon_{k} (n_{k+} + n_{k-}) - \frac{1}{6} g \left(\sum_{k} (n_{k+} - n_{k-}) \right)^{2} . \qquad (7)$$

To find the equilibrium occupation numbers $n_{k\sigma}$, we have to minimize the thermodynamic potential, $\Omega = \langle H \rangle - TS - \zeta N$, where

$$S = -\sum_{k,\sigma} \left[n_{k\sigma} \ln n_{k\sigma} + (1 - n_{k\sigma}) \ln (1 - n_{k\sigma}) \right] , \qquad (8)$$

$$N = \sum_{k,\sigma} n_{k\sigma} \quad , \tag{9}$$

and ζ is the chemical potential. This gives

$$\eta_{k\sigma} = f\left(\epsilon_k - \sigma\lambda\right) \quad , \tag{10}$$

where

4301

$$\lambda = \frac{1}{2}g \sum_{k} (n_{k+} - n_{k-})$$
(11)

and $f(\epsilon) = \{\exp[(\epsilon - \zeta)/T] + 1\}^{-1}$ is the Fermi function. From Eqs. (10) and (11) we find an equation for λ ,

$$\lambda = -\frac{1}{6}g \int [f(\epsilon + \lambda) - f(\epsilon - \lambda)]\nu(\epsilon) d\epsilon , \qquad (12)$$

where $\nu(\epsilon)$ is the density of states in the "normal"

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<u>25</u>

phase $(\lambda = 0)$.

Equation (12) has a trivial solution, $\lambda = 0$, but it can also have other solutions if g is sufficiently large. A nonzero value of λ means that the numbers of particles with positive and negative helicity are not equal, and thus reflectional symmetry is violated. The quasiparticle energy is given by

$$\epsilon_{k\sigma} = \frac{\delta \langle H \rangle}{\delta n_{k\sigma}} = \epsilon_k - \sigma \lambda = \epsilon_k - \lambda (\vec{\sigma} \cdot \hat{k}) \quad . \tag{13}$$

We see that for $\lambda \neq 0$, the band splits into two bands with different helicities. The bottoms of these bands are separated by 2λ . For small λ the two bands overlap, but for sufficiently large λ they can be separated by a gap. If the original band was half full, this corresponds to an insulating state. In general, the broken-symmetric state can be metallic, insulating, semiconducting, or semimetallic, depending on the band structure and on the magnitude of λ . In the case of small λ Eqs. (12) and (13) were obtained in Ref. 1.

At zero temperature, and for a parabolic band with $\epsilon_k = k^2/2m$, Eq. (12) reduces to

$$\lambda/\zeta = \frac{1}{9}g\nu_0[(1+\lambda/\zeta)^{3/2} - (1-\lambda/\zeta)^{3/2}] \quad , \qquad (14)$$

where $\nu_0 = \nu(\zeta)$. It has nonzero solutions only if $g\nu_0 > 3$, i.e., in the case of strong interaction and/or narrow bands. It can be verified that for $g\nu_0 > 3$ there are two nontrivial solutions of equal magnitude and opposite sign and that these solutions provide smaller energy than the normal solution $\lambda = 0$.

The broken symmetry can be restored at sufficiently high temperatures. Assuming that $\lambda, T \ll \zeta$ and $\epsilon_k = k^2/2m$, Eq. (12) gives

$$\lambda^2 = 24\zeta^2 (1 - 3/g\nu_0) - \pi^2 T^2 \quad . \tag{15}$$

The symmetry is restored at $T > T_c$, where

$$T_c^2 = 24\pi^{-2}\zeta^2(1 - 3/g\nu_0) \quad . \tag{16}$$

The phase transition is of the second order. Equation (16) is valid only if $T_c \ll \zeta$, i.e., $(1 - 3/gv_0) \ll 1$. In general case one can expect T_c , λ , and ζ to be of the same order of magnitude.

Let us now discuss the physical effects which are characteristic of the state with broken reflectional symmetry. If a magnetic field \vec{B} is applied to the system, the spins of electrons align with the magnetic field, and since $\langle \vec{\sigma} \cdot \vec{k} \rangle \neq 0$, one could expect an electric current to flow in the direction parallel or antiparallel to \vec{B} . It will be shown, however, that such an effect does not occur in thermal equilibrium.

We shall assume that the quantization of electron orbits in the magnetic field is unimportant. Then the current density equals

$$\vec{j} = e \operatorname{Tr} \sum_{k} \vec{\nabla}_{k} f(\mathcal{S}_{k}) \quad , \tag{17}$$

where e is the electron charge, $\vec{v}_k = \vec{\nabla}_k \delta_k$ is the quasiparticle velocity,

$$\boldsymbol{\delta}_{k} = \boldsymbol{\epsilon}_{k} - \lambda (\,\vec{\sigma} \cdot \hat{k}\,) - \mu (\,\vec{\sigma} \cdot \vec{B}\,) \tag{18}$$

is the quasiparticle energy, and μ is the electron magnetic moment. (Note that \mathscr{S}_k and v_k are spin matrices.) Strictly speaking, \vec{k} in Eq. (18) has to be replaced by $\vec{k} - e\vec{A}/c$, but the additional term does not contribute to Eq. (17), since it can be transformed away by shifting the origin of the \vec{k} space. Integrating by parts we obtain

$$\vec{j} = e \operatorname{Tr} \sum_{k} \vec{\nabla}_{k} \phi(\mathcal{S}_{k}) = 0$$
, (19)

where

$$\phi(\mathcal{S}_k) = \int_{\mu}^{\mathcal{S}_k} f(\epsilon) d\epsilon = -T \ln\left(1 + \exp\frac{\zeta - \mathcal{S}_k}{T}\right) .$$
(20)

Although an electric current parallel to \vec{B} is no longer prohibited by reflectional symmetry, the symmetrybreaking terms in \mathscr{E}_k and \vec{v}_k conspire to make \vec{j} equal to zero.³ On the other hand, the (quasi-) momentum density of electrons is not equal to zero:

$$\vec{\mathbf{P}} = \operatorname{Tr} \sum_{k} \vec{\mathbf{k}} f\left(\boldsymbol{\mathcal{S}}_{k}\right) = \frac{1}{2} n k_{F} \frac{\lambda}{\zeta} \frac{\mu \mathbf{B}}{\zeta} \quad .$$
(21)

Here the last equality corresponds to the case $\epsilon_k = k^2/2m$; λ , $T \ll \zeta$, *n* is the electron density, and $k_F = (2m\zeta)^{1/2}$ is the Fermi momentum. There is no contradiction between (19) and (21), because $\vec{\nabla}_k = \vec{\nabla}_k \mathcal{S}_k \neq \vec{k}/m$. Since the total momentum of electrons plus the lattice is conserved, we expect the whole sample to recoil when the magnetic field is turned on.

An electric current parallel to \vec{B} does occur in a number of nonequilibrium situations. In a timevarying magnetic field, $\vec{B}(t) = \vec{B}e^{-i\omega t}$, the Boltzmann equation can be written as

$$\frac{\partial n_k}{\partial t} = -\frac{n_k - f\left(\mathcal{S}_k\right)}{\tau_k} \quad , \tag{22}$$

where n_k is the electron distribution function and \mathcal{S}_k is given by Eq. (18) with $\vec{B} = \vec{B}(t)$; n_k and \mathcal{S}_k are spin matrices. We shall assume for simplicity that the relaxation time τ_k is a *c* number and that it depends only on $\epsilon_k = k^2/2m$. On the left-hand side of Eq. (22) we have neglected terms corresponding to the magnetic part of the Lorentz force and to the spin precession around the direction of $(\lambda \hat{k} + \mu \vec{B})$. These effects are unrelated to the alignment of $\vec{\sigma}$ with \vec{B} and of $\vec{\sigma}$ with \vec{k} and thus do not contribute to the current in the approximation linear in λ and \vec{B} . Introducing

$$n_{k}^{(1)} = n_{k} - f(\boldsymbol{\mathcal{S}}_{k}) << n_{k}$$
(23)

4302

$$n_{k}^{(1)} = \tau_{k} \mu \left(\vec{\sigma} \cdot \frac{d\vec{\mathbf{B}}}{dt} \right) f'(\boldsymbol{\epsilon}_{k} - \lambda \, \vec{\sigma} \cdot \hat{k}) \quad . \tag{24}$$

The current density is given by

$$\vec{j} = e \operatorname{Tr} \sum_{k} \vec{\nabla}_{k} n_{k}^{(1)}$$
$$= e \mu \operatorname{Tr} \sum_{k} \tau_{k} \left(\vec{\sigma} \cdot \frac{d\vec{B}}{dt} \right) \vec{\nabla}_{k} f \left(\epsilon_{k} - \lambda \vec{\sigma} \cdot \hat{k} \right) \quad . \tag{25}$$

Integrating by parts and assuming that $\lambda, T \ll \zeta$ we find

$$\vec{j} = -\frac{1}{2} en v_F \frac{\lambda}{\zeta} \frac{d\tau}{d\zeta} \mu \frac{d\vec{B}}{dt} , \qquad (26)$$

where $v_F = k_F/m$ is the Fermi velocity and $d\tau/d\zeta = (d\tau_k/d\epsilon_k)|_{\epsilon_k=\zeta}$. Although Eq. (26) was derived for $\lambda \ll \zeta$, it should give a correct order of magnitude of the current for $\lambda \sim \zeta$. An experimental observation of the symmetry-violating current (26) may turn out to be very difficult, because of the presence of much greater currents induced by a time-varying magnetic field.

A current parallel to \overline{B} can also occur in a constant magnetic field in the presence of electromagnetic radiation. Since light practically does not penetrate in metals, we consider a semiconductor with $\omega_p < \omega$ $< \delta$, where ω is the frequency of light, ω_p is the plasma frequency, and δ is the gap between the valence and conduction bands. We assume for simplicity that free-charge carriers are present only in one of the bands and that the bands of opposite helicity are completely separated. The corresponding Boltzmann equation is

$$\frac{\partial n_k}{\partial t} + e\vec{E}\frac{\partial n_k}{\partial \vec{k}} = -\frac{n_k - n_k^{(0)}}{\tau} , \qquad (27)$$

where $n_k^{(0)} = \frac{1}{2} (1 \pm \vec{\sigma} \cdot \hat{k}) f(\epsilon_k - \mu \vec{\sigma} \cdot \vec{B})$. A nonzero symmetry-violating contribution to the current appears only in the second order of perturbation theory

in Ē:

$$j_i = \frac{e^2}{\omega^2 + \tau^{-2}} \langle E_m E_n \rangle_{\rm av} \operatorname{Tr} \sum_k v_i \frac{\partial^2 n_k^{(0)}}{\partial k_m \partial k_n} , \qquad (28)$$

where we have assumed that $\tau = \text{const.}$ It is easily seen that the current (28) vanished for a parabolic band. We therefore take

$$\epsilon_k = \frac{k^2}{2m} + \frac{1}{4!}\beta k^4 \quad . \tag{29}$$

For a nondegenerate semiconductor with $\omega \tau >> 1$ and with the light flux parallel to the magnetic field, Eqs. (28) and (29) give⁴

$$\vec{\mathbf{j}} = \pm \frac{32}{9} \frac{e^2 \beta n I}{c \, v_T \omega^2} \mu \vec{\mathbf{B}} \quad , \tag{30}$$

where *n* is the density of charge carriers, v_T $=(8T/\pi m)^{1/2}$ is the thermal velocity, and $I = c \langle E^2 \rangle_{av} / 4\pi$ is the light intensity inside the semiconductor. To estimate the current (30), we take $\beta \sim (m^2 \Delta)^{-1}$, where $\Delta \sim 1$ eV is the bandwidth $n \sim 10^{18} \text{ cm}^{-3}$, $T \sim 300 \text{ K}$, $\omega \sim 3 \times 10^{15} \text{ s}^{-1}$, $I \sim 10^2$ W/cm² (such light intensities can be produced using a laser), and $B \sim 10^4$ G. This gives $j \sim 10^{-8}$ A/cm². Observationally, the symmetry-violating current can be obscured by the "photon drag" of the charge carriers (Dember effect). To get around this difficulty, one can use the fact that if \vec{B} slowly (to avoid induced currents) changes in time with a frequency ω_0 , then all reflectionally symmetric contributions to \overline{j} will change with frequency $2\omega_0$, while the frequency of the current (30) will be ω_0 .

Other symmetry-violating effects including electron polarization in autoelectronic emission from metals and the rotation of the plane of polarization of light. These and other effects will be discussed elsewhere. It is interesting that, although the symmetry violation can be strong ($\lambda \sim \zeta$), the associated physical effects are extremely small. For this reason, spontaneous violation of reflectional symmetry may have passed unnoticed even in well-studied materials, and its experimental detection may prove to be a challenging task for experimentalists.

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⁴In the derivation of Eq. (30) we have neglected Landau diamagnetism. This can be justified in the case of narrow bands. The energy quantum for orbital quantization is $\Delta \epsilon_{orb} = e\hbar/mc$, while for spin quantization it is $\Delta \epsilon_{spin}$ $= e\hbar/m_ec$, where *m* and m_e are effective mass and electron mass, respectively. For $m >> m_e$, we have $\Delta \epsilon_{orb} << \Delta \epsilon_{spin}$. In any case, we expect Eq. (30) to give a correct order of magnitude of the effect.

4303