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INVERSION ASYMMETRY EFFECTS ON OSCILLATORY MAGNETORESISTANCE IN HgSe †

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A beat frequency in the oscillatory magnetoresistance of zincblende HgSe is interpreted as arising from the inversion-asymmetry splitting, which is shown to be about 0.007 eV at the Fermi level appropriate to 1×10^{18} electrons/cm^3.

The space group of the diamond lattice has an inversion symmetry operation which requires that $E(\vec{k})$ be twofold degenerate for all $\vec{k}$. The zincblende lattice results from replacing the two group-IV atoms of the diamond lattice basis with one group-III atom and one group-V atom (or a group-II and a group-VI atom), and the inversion symmetry is lost. If the zincblende material has a finite spin-orbit splitting, $E(\vec{k})$ will no longer be twofold degenerate at a general value of $\vec{k}$. Although the theoretical existence of this inversion-asymmetry splitting has been recognized for some time,[1] the small size of the splitting has made it difficult to observe experimentally. Recently, Robinson[2] reported results of cyclotron resonance on p-type InSb which, he argued, required the inversion-asymmetry splitting for interpretation. In this Letter we propose that the Shubnikov–de Haas (SdH) measurements of Whitsett[3] on n-type HgSe quite strikingly demonstrate these zincblende splittings. We first rule out another possible explanation of Whitsett's results and then show how to find the orbits which give the SdH frequencies. An interesting situation occurs when the magnetic field, $\vec{B}$, is parallel to a $\langle100\rangle$ direction. The $\langle100\rangle$ zero-field orbits are quenched by magnetic-field–induced splittings in a fashion which is the reverse of magnetic breakdown. By comparing the SdH frequencies with those computed from the theoretical E vs $\vec{k}$ we find values of the inversion-asymmetry splitting for HgSe.

Whitsett's results show that the conduction-band cross-sectional area is only weakly dependent on the direction of $\vec{B}$ with respect to the crystalline axes, as expected for a band with a minimum at $\vec{k}=0$. However, at electron concentrations of $\sim1\times10^{18}$ cm^{-3} and higher, a beat frequency is found for $\vec{B}$ along all directions in the $(1\bar{1}0)$ plane except $\langle110\rangle$. These effects are reproducible from sample to sample and we have verified Whitsett's results in our laboratory.

Although the details of the HgSe band structure have not been conclusively established, it is expected that the conduction band was either p-like Γ_8 symmetry as α-Sn or s-like Γ_6 symmetry as InSb, and it is possible to treat these two cases together. Kane has found the energy for either a Γ_6 or Γ_8 band to be[4]

$$E^{\pm}=E'+(\hbar^2/2m_0+a^2A'+b^2M+c^2L')k^2 + (b^2-2c^2)(L-M-N)f_1(\vec{k})\pm\sqrt{2}\,ab\beta f_2(\vec{k}), \quad (1)$$

where

$$f_1(\vec{k}) = (k_x^2 k_y^2 + k_x^2 k_z^2 + k_y^2 k_z^2)/k^2$$

and

$$f_2(\vec{k}) = [k^2(k_x^2 k_y^2 + k_x^2 k_z^2 + k_y^2 k_z^2) - 9k_x^2 k_y^2 k_z^2]^{1/2} k.$$

E' is the conduction-band eigenvalue resulting from the diagonalization of the Hamiltonian which includes the $\vec{k}\cdot\vec{p}$ and the largest spin-orbit interaction terms between an s-like (Γ_6) and p-like ($\Gamma_8 + \Gamma_7$) basis. a, b, and c are normalized coefficients which give the admixture of s- and p-state basis in the eigenvector corresponding to E'. (At $\vec{k} = 0$ for a Γ_6 band, $a = 1$ and $b = c = 0$, while for a Γ_8 band $a = 0$, $b = \sqrt{\frac{1}{3}}$ and $c = \sqrt{\frac{2}{3}}$. In either case there is rapid admixing of the s and p components off $\vec{k} = 0$ for small-gap materials such as HgSe.) A', L, M, N, L', and β (Kane's B) are parameters which describe the interaction between far-removed conduction- and valence-band edges and the s- and p-like bands.

E' is spherically symmetric and therefore the only angular dependence of $E^{\pm}$ comes from the terms $f_1(\vec{k})$ and $f_2(\vec{k})$. The term $f_1(\vec{k})$ adds a cubic warping to the energy surfaces and the term $f_2(\vec{k})$ gives the inversion-asymmetry splitting ($\beta = 0$ for the diamond lattice). For small k the produce ab is proportional to k and the splitting is proportional to k^3. For a Γ_8 band there is also a splitting term linear in k which we omit, since for Fermi energies much larger than the inversion-asymmetry splittings it has the same symmetry as the β or k^3 term. The relative importance of these terms could be decided by measuring the E or k dependence of the splitting. The fact that the beating is seen only in the higher concentration samples suggests that the k^3 term is more important.

The higher band coefficient (L-M-N) is positive for Ge and InSb and is expected to be the same for HgSe. $2c^2$ is greater than b^2 and thus the coefficient multiplying $f_1(\vec{k})$ is negative. If L-M-N is sufficiently large the warping can cause the maximum cross-sectional area perpendicular to k_3 to occur off $k_3 = 0$ for $k_3 \parallel \langle 111\rangle$ or $\langle 100\rangle$. (We use k_3 as the direction of $\vec{B}$.) In this case a local minimum in cross-sectional area occurs at $k_3 = 0$, and for $\vec{B}$ in these directions the two extremal areas give rise to two SdH frequencies which add together in the conductivity to give an average-frequency term modulated by a beat-frequency term. In principle, then, the warping term could explain the orientation dependence of the beating in HgSe. However, a quantitative examination reveals two reasons for rejecting this explanation. First, to get extremal areas off $k_3 = 0$ the warping must be 3 to 6 times larger than in the other diamond and zincblende semiconductors, but the warping is found to vary slowly from material to material in this semiconductor family. The second and more convincing argument is that the required warping causes more than a 20% difference in the sum-frequency periods between $\vec{B}$ along $\langle 111\rangle$ directions, while Whitsett observed less than a 7% variation at maximum and usually only a 3% variation. For these reasons we reject the warping as the explanation of the beating and turn our attention to the inversion-asymmetry splitting term.

Figure 1 shows the constant-energy contours of the split bands in the $k_3 = 0$ plane for k_3 or $\vec{B}$ parallel to $\langle 100\rangle$, $\langle 110\rangle$, and $\langle 111\rangle$. The splitting vanishes for $\vec{k}$ along the $\langle 111\rangle$ and $\langle 100\rangle$ directions. The case for $\vec{B}$ along $\langle 111\rangle$ is uncomplicated: There are two unambiguous orbits and areas and each contributes a SdH frequency. For the other two directions it is not clear which are the proper orbits and Fig. 1 certainly does not suggest that two extremal areas arise for $\vec{B}$ along $\langle 100\rangle$ and only one for $\vec{B}$ along $\langle 110\rangle$,

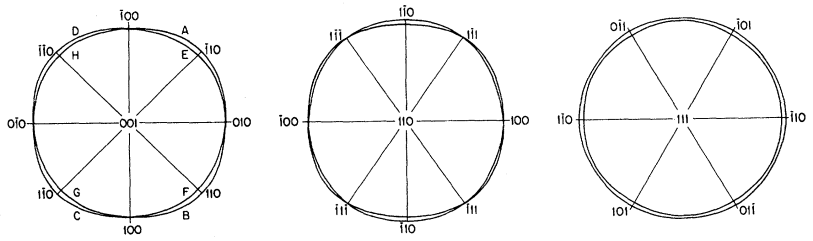

FIG. 1. Constant-energy surfaces with inversion-asymmetry splitting for $k_3 = 0$, with k_3 along [001], [110], and [111] directions.

as demanded by the beat-frequency pattern. Before tackling this difficulty we look at the size of the zincblende splitting needed to give the observed beat frequencies. With the aid of a computer two values of $\vec{k}$ are found from Eq. (1) for a given Fermi energy, E_F, and orientation, θ, and then the angular integration, $\frac{1}{2}\oint k_\pm^2(E_F, \theta)d\theta$, is performed to give the areas of the sections shown in Fig. 1. The details of this computation, which uses energy band parameters which are known for HgSe and values typical of Ge and InSb for the remainder, will be given elsewhere. We find β to be about 6 units of $\hbar^2/2m_0$ or $\sim 2\times 10^{-15}$ eV cm^2 for a Γ_8 conduction band and twice as large for a Γ_6 conduction band. With 1×10^{18} electrons/cm^3 ($E_F = 0.13$ eV), the maximum splitting of the bands ($\vec{k} \parallel \langle 110\rangle$) is ~0.007 eV. Kane has estimated that this splitting might be 0.1 eV at the Fermi level for 10^{19} electrons/cm^3 in InSb. With only this for comparison, the size of the HgSe splitting seems reasonable, and we return to the problem of finding the proper orbits.

First, for simplicity we drop the nonparabolicity and warping from Eq. (1) and write a 2 ×2 Hamiltonian:

$$H = \frac{\hbar^2 k^2}{2m^*} + \frac{\hbar\omega_s \vec{\sigma}\cdot\vec{B}}{2|B|} + \frac{\gamma\hbar^2}{2m^* k_F}[(\sigma_x k_y - \sigma_y k_x)k_x k_y + (\sigma_y k_z - \sigma_z k_y)k_y k_z + (\sigma_z k_x - \sigma_x k_z)k_z k_x], \tag{2}$$

where the σ's are the 2×2 Pauli matrices and k_F is the radius of the Fermi sphere if $\gamma = 0$. We have included a spin term with Zeeman splitting ω_s. The third term in Eq. (2) is invariant under the symmetry operations of the zincblende lattice but not invariant under inversion. The parameter γ equals $\sqrt{2}ab\beta m^*/\hbar^2$ and has the significance that γE_F is the maximum splitting at the Fermi energy, E_F. The Hamiltonian in Eq. (2) has eigenvalues, for $\vec{B} = 0$,

$$E = \frac{\hbar^2 k^2}{2m^*} \pm \frac{\gamma\hbar^2}{2m^*} f_2(\vec{k}). \tag{3}$$

For a finite magnetic field we regard $\vec{k}$ as the operator $\hbar\vec{k} = \vec{p} + e\vec{A}/c$, where $\vec{p} = -i\hbar\nabla$ and $\vec{A}$ is the vector potential. The components of $\vec{k}$ now no longer commute (see below) but we shall ignore the commutator in the term of order γ which is already small. In order to deal with the three directions of of interest it is convenient to express Eq. (2) in terms of $\vec{k}$ and σ components of a coordinate system in which $\vec{B}$ is parallel to k_3 and lies in the $(1\bar{1}0)$ plane[5]:

$$\begin{aligned} k_x &= 2^{-1/2}(k_1\cos\theta - k_2 + k_3\sin\theta), \\ k_y &= 2^{-1/2}(k_1\cos\theta + k_2 + k_3\sin\theta), \\ k_z &= -k_1\sin\theta + k_3\cos\theta, \end{aligned} \tag{4}$$

where θ is the angle between k_3 and k_z. The same transformation applies to the σ's. If Eq. (2) is transformed and k_3 set equal to 0 the following are found:

$$\vec{B} \parallel \langle 100\rangle: \quad H = \frac{\hbar^2 k^2}{2m^*} + \frac{\hbar\omega_s\sigma_3}{2} + \frac{\gamma\hbar^2}{2m^* k_F}(\sigma_1 k_2 - \sigma_2 k_1)\frac{(k_1^2 - k_2^2)}{2},$$

$$\vec{B} \parallel \langle 110\rangle: \quad H = \frac{\hbar^2 k^2}{2m^*} + \frac{\hbar\omega_s\sigma_3}{2} + \frac{\gamma\hbar^2}{2m^* k_F}\sigma_3 k_2\frac{(2k_1^2 - k_2^2)}{2},$$

$$\vec{B} \parallel \langle 111\rangle: \quad H = \frac{\hbar^2 k^2}{2m^*} + \frac{\hbar\omega_s\sigma_3}{2} + \frac{\gamma\hbar^2}{2m^* k_F}\left[\left(\frac{2}{3}\right)^{1/2}\sigma_3 k_2\frac{(3k_1^2 - k_2^2)}{2} - \left(\frac{1}{3}\right)^{1/2}\frac{(k_1^2 + k_2^2)}{2}(\sigma_1 k_2 - \sigma_2 k_1)\right]. \tag{5}$$

For $\vec{B}$ along $\langle 111\rangle$ we have already argued that a semiclassical method based on Eq. (3) is reasonable, giving two slightly differing SdH frequencies. For the $\langle 110\rangle$ case, Eq. (5) shows that H is diagonal

and the eigenvalues are those of

$$H^{\pm}=\frac{\gamma\hbar^2k^2}{2m^*}\pm\left[\frac{\gamma\hbar^2}{2m^*k_F}k_2\frac{(2k_1^2-k_2^2)}{2}+\frac{\hbar\omega_s}{2}\right]. \tag{6}$$

These equations can now be treated semiclassically. The orbits in this case trace out equal areas and thus contribute only one SdH frequency. This is in agreement with the experimental result.

For $\vec{B}\parallel\langle 100\rangle$ the situation is more complicated. We call the second part of the Hamiltonian H' and wish to transform to a representation in which H' is diagonal. In matrix form,

$$H'=\frac{\gamma\hbar^2}{2m^*k_F}\frac{(k_1^2-k_2^2)}{2}i\begin{bmatrix}0 & (k_1-ik_2)\\ -(k_1+ik_2) & 0\end{bmatrix}. \tag{7}$$

If we ignore the fact that k_1 and k_2 do not commute, and write $k_1\pm ik_2=k\exp[\pm i\varphi]$, we can diagonalize Eq. (7) by means of the unitary transformation

$$U=\begin{bmatrix}\lambda^* & -\lambda^*\\ \lambda & \lambda\end{bmatrix}, \tag{8}$$

where $\lambda=2^{-1/2}\exp[i(\frac{1}{2}\varphi-\frac{1}{4}\pi)]$. With $k\simeq k_F$, this gives

$$\bar{H}'=U^{\dagger}H'U=\frac{\gamma\hbar^2}{2m^*}\frac{(k_1^2-k_2^2)}{2}\sigma_3. \tag{9}$$

In transforming the first term of H, however, we must consider the commutation relation $[k_1,k_2]=eB/i\hbar c$. We use the creation and destruction operators for harmonic oscillator wave functions,

$$a^{\dagger}=\left(\frac{\hbar c}{2eB}\right)^{1/2}(k_1+ik_2),$$

$$a=\left(\frac{\hbar c}{2eB}\right)^{1/2}(k_1-k_2),$$

which have the property $a^{\dagger}a=n$, where n is the order of the harmonic-oscillator wave function. We now define $e^{i\varphi}$ as the operator $n^{-1/2}a^{\dagger}$, valid for large n, and $e^{-i\varphi}$ as $an^{-1/2}$. While $e^{i\varphi}$ and $e^{-i\varphi}$ commute with each other they do not commute with n; in fact, $ne^{i\varphi}=e^{i\varphi}(n+1)$. Using this we transform the first two terms of H and combine with Eq. (9) to obtain

$$\bar{H}=\begin{bmatrix}\frac{\hbar^2k^2}{2m^*}+\frac{\gamma\hbar^2}{2m^*}\frac{(k_1^2-k_2^2)}{2} & \frac{\hbar(\omega_c-\omega_s)}{2}\\ \frac{\hbar(\omega_c-\omega_s)}{2} & \frac{\hbar^2k^2}{2m}-\frac{\gamma\hbar^2}{2m^*}\frac{(k_1^2-k_2^2)}{2}\end{bmatrix}, \tag{10}$$

where $\omega_c=eB/m^*c$ is the cyclotron frequency. We notice that terms of order $n\hbar\omega_c$, $\hbar\omega_c$, and $\gamma n\hbar\omega_c$ have been kept, but terms of order $\gamma\hbar\omega_c$ have been kept, but terms of order $\gamma\hbar\omega_c$ have been dropped. If the more general terms from Eq. (1) had been used, these would replace $\hbar^2k^2/2m^*$ in Eq. (10) and $\hbar(\omega_c-\omega_s)$ would be replaced by the cyclotron energy and spin splitting appropriate to the Fermi level.

Thus we see that at zero field the orbits for $\vec{B} \parallel \langle 100 \rangle$ cross as in Fig. 1 and trace out equal areas. However, unlike the case of $\vec{B} \parallel \langle 110 \rangle$, there is a coupling between the orbits at finite fields and if this is large enough the electrons follow the outer and inner orbits of Fig. 1 and there are two extremal areas and two SdH frequencies, as observed.

Close to the crossover point the Hamiltonian of Eq. (10) is similar to that which Blount uses in his treatment of magnetic breakdown.[6] He writes

$$H = \begin{bmatrix} \vec{k}\cdot\vec{v}_1 & \Delta \\ \Delta & \vec{k}\cdot\vec{v}_2 \end{bmatrix}, \tag{11}$$

where $\vec{v} = \hbar^{-1}\nabla_k E$, evaluated at the crossover points, and Δ is a small perturbation which keeps the bands from crossing. In the phenomenon of magnetic breakdown a sufficiently strong field induces transitions across the gap Δ. Our situation is, in a sense, just the opposite of magnetic breakdown. The quantity $\frac{1}{2}\hbar(\omega_C - \omega_S)$ takes the place of Δ, and we do not have a zero-field energy gap which is jumped by the magnetic field but a field-induced energy gap which forces the electrons to change from their zero-field orbits. Blount's results can be interpreted in terms of a Δ-induced switching coefficient Q^2, or probability of jumping between $\Delta = 0$ orbits at the points of close approach, which is given by $Q^2 = 1 - \exp(-s^2)$, with $s^2 = 2\pi\Delta^2\hbar c/[eB\cdot(\vec{v}_1 \times \vec{v}_2)]$. For our case s^2 becomes $\pi\hbar(\omega_C - \omega_S)/4E_F\gamma$, i.e., the ratio of a magnetic splitting at the Fermi level to the maximum inversion-asymmetry splitting.

As discussed above, we find $\gamma E_F \simeq 0.007$ eV for $n = 1\times10^{18}$ cm^{-3}. At 10 kG, the region of magnetic field where the beating is first observed, the cyclotron energy at the Fermi energy is slightly greater than 0.002 eV. The g factor is negative for both Γ_6 and Γ_8 conduction bands and this enhances the reverse breakdown effect by adding the spin splitting, $\simeq$0.001 eV, to $\hbar\omega_C$. Thus s^2 is about 0.3. Actually, if s^2 were quite large we could be sure that reverse breakdown would be complete. However, the prediction is for an incomplete breakdown. Such a situation can be analyzed in terms of a Pippard-type network. We shall not go into details but the result is an amplitude function,

$$a(B) = 2\{\exp(-s^2) - [1-\exp(-s^2)]\cos(\hbar c\alpha/4eB)\}^2 - 1,$$

modulating the average period, where α is the maximum area difference in Fig. 1(a). If s^2 is small all that results is a slight reduction in amplitude with a period $8\pi e/\alpha\hbar c$, or 4 times the expected beat period. As s^2 increases nodes develop (at $s^2 = 0.16$) and then more nodes, until for $s^2 \to \infty$ the spacing of the nodes is $2\pi e/\alpha\hbar c$. This model thus predicts nodes in the present experimental situation, but not of the frequency we at first expected. Physically, these longer beat periods correspond to intermediate orbits; thus the small-s^2 beat period would correspond to beating A_0, the zero-field area, $AFCH$ in Fig. 1, against $A_0 + \frac{1}{4}\alpha$, which would result from an electron which switched at two junctions but not at the other two, (i.e., orbit $ABCH$ in Fig. 1).

It should be noted that experimentally a complete period was not observed for the $\langle 100 \rangle$ direction, and that minima rather than nodes were sometimes observed. Therefore, it is possible that the partial breakdown is occurring. However, it would also seem that the condition for reverse breakdown to be complete, i.e., the magnetic splitting to be of the order of the inversion-asymmetry splitting, would tend to invalidate the WKB-type arguments which go into the standard treatments of magnetic breakdown. Thus the orbits we are considering never get far away from each other as they would in a metal. It would be beneficial if more exact methods could be employed, such as possibly solving the coupled equations in Eq. (2) exactly.

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