InAs to that of InSb, the theory presented may also be applied to Geist's susceptibility data on InAs.[23] As expected, there is a qualitative similarity between the data on these two substances.

CONCLUSION

The results of measurements on the carrier susceptibility in n-InSb show that the susceptibility departs appreciably from that of a parabolic band. The essential feature of the observed susceptibility is that it increases with increasing carrier density at low carrier densities and decreases at high carrier densities. A theoretical analysis based on current ideas about the band structure of InSb shows that at low carrier densities the interaction between the valence band and the conduction band is the principal contributor to the susceptibility. This interaction alone cannot explain the observed behavior of χ at the higher densities. The effect of higher bands is estimated to be of sufficient magnitude to account for the decrease of the susceptibility at the higher densities. Within the limitation resulting from the approximate computation of the higher band interactions, the observed susceptibility appears consistent with Kane's band-structure calculation.

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[23] D. Geist, Z. Naturforsch. **13a**, 699 (1958).

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Energy Levels of Conduction Electrons in a Magnetic Field

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The energy levels of an electron in a periodic potential and a constant magnetic field are found as the solutions to a secular determinant when the following approximations are made: (a) the energy band of interest is spherically symmetric and (b) lattice broadening of the levels is neglected. Inclusion of spin-orbit coupling gives the g factor as function of position in the band. Perturbation theory is used to treat the effect on the free energy of small departures of the band from spherical symmetry.

INTRODUCTION

THIS paper is concerned with the determination of the energy levels of an electron in a periodic potential and an applied constant magnetic field. The problem is formulated in the Luttinger-Kohn[1] representation and since this representation has been used in several papers dealing with the magnetic properties of conduction electrons, we first review briefly this previous work.

The treatments of Luttinger and Kohn[1] and Kjeldaas and Kohn[2] for nondegenerate bands are based on an expansion in powers of k_0, the wave-vector at the Fermi surface and thus are useful only if this expansion converges fast enough. Considering the magnetic levels of the valence band of germanium, Luttinger[3] included the interactions[4] between the valence band and other bands to order k^2. When the band structure coefficients were such that the valence band was spherically symmetric, the magnetic levels could be obtained exactly. On the other hand, in the case of two-dimensional graphite the energy is not an analytic function of $\mathbf{k}$ at $k=0$ so that an expansion in powers of k is impossible. For this case, McClure[5] obtained the magnetic levels for any k exactly as far as the magnetic interactions are concerned; however other approximations were made in the calculation.

It is the purpose of this paper to extend these results by pointing out that in the approximation of spherical bands the existence of a selection rule in the interband matrix elements of the velocity makes it possible to obtain the energy levels exactly[6] for arbitrary k. Since energy bands are not in general spherical, the levels thus obtained are strictly speaking, not those of an electron in a lattice, except in the case of cubic symmetry with only s and p bands interacting. Rather they are the levels of a model which is an approximation to substances with nearly spherically symmetric energy bands, such as the alkali metals or semiconductors such as InSb.[7] The corrections to the energy

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[1] J. M. Luttinger and W. Kohn, Phys. Rev. **97**, 869 (1955).

[2] T. Kjeldaas and W. Kohn, Phys. Rev. **105**, 806 (1957).

[3] J. M. Luttinger, Phys. Rev. **102**, 1030 (1956).

[4] The expression "interaction between bands" refers to the off-diagonal elements in the hamiltonian matrix, resulting from the interband matrix elements of the velocity between the L. K. states.

[5] J. W. McClure, Phys. Rev. **104**, 666 (1956).

[6] Except for the lattice broadening which is neglected; see below.

[7] Treated in R. Bowers and Y. Yafet, preceding paper [Phys. Rev. **115**, 1165 (1959)].

levels arising from the departure from sphericity cannot be treated by perturbation theory because the level splittings of the quantized levels are very small. However the corrections to the nonoscillatory part of the free energy can be obtained by perturbation theory, as seen below, so that the spherical model can provide a consistent procedure for approximating some of the magnetic properties of solids and in particular the susceptibility. Furthermore the simplicity of the solutions which it gives, both for degenerate and nondegenerate bands and including all the interband effects, makes this model worthy of consideration.

The inclusion of spin-orbit coupling offers no difficulty so that the g factor for spin resonance can be found as function of position in the band. The method of obtaining the energy levels and wave functions will be given first for the case of no spin-orbit coupling, the effect of the latter will be considered next and finally the perturbation treatment of a departure from sphericity will be sketched.

ENERGY LEVELS AND WAVE FUNCTIONS

The crystal Hamiltonian $H=p^2/2m+V(\mathbf{r})$ is assumed to have space inversion symmetry. We choose the gauge $\mathbf{A}=(0,\mathcal{H}x,0)$ for the magnetic field $\mathcal{H}$. The representative of the Hamiltonian in the L. K. states $\chi_{\mu,\mathbf{k}}(\mathbf{r})=u_\mu(\mathbf{r})e^{i\mathbf{k}\cdot\mathbf{r}}$ is given, in atomic units,[8] by[1]

$$H_{\mu'\mathbf{k}';\mu''\mathbf{k}''}=E_{\mu'}\delta_{\mu'\mu''}\delta(\mathbf{k}'-\mathbf{k}'')+\sum_i (p_i)_{\mu'\mu''}\langle\mathbf{k}'|\bar{k}_i|\mathbf{k}''\rangle +\sum_i \tfrac{1}{2}\delta_{\mu'\mu''}\langle\mathbf{k}'|\bar{k}_i^2|\mathbf{k}''\rangle. \quad (1)$$

Here μ' is the band index, $E_{\mu'}$ is the energy at $k=0$, and the $(p_i)_{\mu'\mu''}$ are the interband matrix elements of the i component of momentum. The operators $\bar{k}_i$ are given by $\bar{k}_x=k_x$, $\bar{k}_y=k_y+is\partial/\partial k_x$, $\bar{k}_z=k_z$ with $s=e\mathcal{H}/\hbar c$ and their representatives $\langle\mathbf{k}'|\bar{k}_i|\mathbf{k}''\rangle$ are taken over plane-wave states.

The eigenvalue equation for (1) is an infinite set of coupled differential equations for the components of the wave function in the L. K. states. These components are clearly of the form $\delta(k_y-k_y')\delta(k_z-k_z')F_{\mu;n,k_y',k_z'}(k_x)$, where n is the quantum number for the degree of freedom k_x; the $F_\mu(k_x)$ obey the relations

$$(E_{\mu'}+\tfrac{1}{2}\bar{k}^2-\lambda)F_{\mu'}(k_x)+\sum_{\mu''\neq\mu'} p_{\mu'\mu''}{}^{(i)}\bar{k}_iF_{\mu''}(k_x)=0. \quad (2)$$

In solving (2) we shall disregard the broadening of the magnetic levels caused by the discreteness of the lattice[9]; as long as the electron distribution does not touch the zone boundaries (which is a requisite of the spherical approximation) the effect of broadening should be negligible.

Formally, broadening is neglected by disregarding the identity between two $\chi_{\mu',\mathbf{k}}(\mathbf{r})$ differing by a reciprocal lattice vector and imposing as boundary conditions on the $F_\mu(k_x)$, the condition of being normalizable in unbounded k_x, k_y space.

When we neglect broadening the energy levels of (2) are seen to be independent of the value of k_y' since a k_x-dependent phase factor $\exp(ik_y'k_x/s)$ multiplying the wave function $F_\mu(k_x)$ can be used to eliminate k_y' from (2). Therefore k_y' is taken equal to zero in which case the interband terms of (2) can be written as

$$[(p_+)_{\mu'\mu''}\bar{k}_-+(p_-)_{\mu'\mu''}\bar{k}_++(p_z)_{\mu'\mu''}k_z]F_{\mu''}(k_x), \quad (3)$$

with $p_\pm=\frac{1}{2}(p_x\pm ip_y)$ and $\bar{k}_\pm=k_x\mp s\partial/\partial k_x$. For a given pair (μ',μ'') in general all three p_+, p_-, p_z may have a nonvanishing matrix element.

We now make the spherical approximation, assuming that the $u_\mu(\mathbf{r})$ are given by $u_{t,l,m}=R_t(r)Y_{l,m}(\theta,\varphi)$ where $R_t(r)$ is a radial function for the band t and $Y_{l,m}$ is the spherical harmonic for angular momentum l and a component of angular momentum m along the magnetic field. With $\mu'=(t',l',m')$ and writing the momentum in spherical coordinates, it is seen that the matrix elements of $p_\pm$, p_z do not vanish only for $m'=m''\pm1$ and $m'=m''$, respectively. Therefore in each of the equations (2), only one of $\bar{k}_+$, $\bar{k}_-$ or k_z acts on $F_{\mu''}$, $\mu''\neq\mu'$ while only $\bar{k}^2$ operates on the inband part $F_{\mu'}$. Finally we notice that $\bar{k}_+$, $\bar{k}_-$, k_z and $\bar{k}^2$, acting on the harmonic oscillator function $\Phi_n(k_x/s^{\frac{1}{2}})$ of the variable $(k_x/s^{\frac{1}{2}})$, give again a single harmonic oscillator function with quantum number $n+1$, $n-1$, n, and n, respectively. It follows that the solutions of (2) are given by

$$\begin{aligned} F_{\alpha;n,0,k_z'}{}^{(t',l',m')}&=C_\alpha{}^{(t',l',m')}(n,k_z',s)\Phi_{n-m'}(k_x/s^{\frac{1}{2}}), \\ &\qquad\qquad n\geqslant m' \quad (4)\\ &=0,\quad n<m' \end{aligned}$$

where the index α denotes the band. A special case of the solution (4) was obtained by Luttinger,[3] to order k^2, in the spherical approximation to the valence band levels in germanium.

For computational purposes it is necessary to limit the number of L. K. states used in obtaining the matrix of H. Suppose that we are interested in the band (t,l,m) for the values of $m=-l$ to $m=+l$, and let N be the number of L. K. states of different energies which it is sufficient to include for the determination of the energy $\lambda_{t,l,m}{}^{(0)}(k^2)$ in the absence of the field to a desired accuracy. Then the solution (4) with the matrix elements

$$(\Phi_{n-m''\pm1},\bar{k}_\pm\Phi_{n-m''})=s^{\frac{1}{2}}[2n+1-(m'+m'')]^{\frac{1}{2}} \quad (5)$$

gives a secular determinant of order $\nu=\sum_{t'=1}{}^N(2l_{t'}+1)$, whose solution gives the energy levels $\lambda_\alpha(k_z'^2,n,s)$ [10] and the coefficients $C_\alpha{}^{(t',l',m')}$. The spherical approximation

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[8] Atomic units, $e=\hbar=m=1$ are used throughout this paper.

[9] A. D. Brailsford, Proc. Phys. Soc. (London) **A70**, 275 (1957); W. Kohn, Proc. Phys. Soc. (London) **72**, 1147 (1958).

[10] E. I. Blount has pointed out (private communication) that even without the spherical approximation and quite generally, the set (2) may be immediately converted into an infinite set of algebraic equations by expanding the $F_\mu(k_x)$ into the complete set of harmonic oscillator functions of $(k_x/s^{\frac{1}{2}})$ and using (5).

has therefore enabled us to reduce the set of differential equations to a finite (for finite N) set of algebraic linear equations.

The wave function in $\mathbf{r}$ space, neglecting effects of the same order as those causing broadening, is given by the sum of the Fourier transforms of the components of the wave function in $\mathbf{k}$ space, and since the transform of $\Phi_n(k_x/s^{\frac{1}{2}})$ is $(-i)^n\Phi_n(xs^{\frac{1}{2}})$, we obtain

$$\psi_{\alpha;n,k_y,k_z}(\mathbf{r})=e^{i(k_yy+k_zz)}\sum\nolimits_\mu(-i)^{n-m}C_\alpha{}^{(\mu)} \times\Phi_{n-m}[(x+k_y/s)s^{\frac{1}{2}}]u_\mu(\mathbf{r}). \quad (6)$$

Thus in the spherical approximation the wave function has a rather simple form, being the sum of ν terms, each of which is the product of a periodic part $C_\alpha{}^{(\mu)}u_\mu(\mathbf{r})$ characteristic of the periodic potential and an envelope function which is the same as the wave function for a free particle.

In calculations of the magnetic susceptibility the energy levels are needed only to order s^2; in the rest of this section we shall show that the secular equation which must be solved may then be reduced to that in the absence of a field by expanding the secular determinant in powers of s and we shall obtain the form of this expansion.

We consider first the secular equation for $\mathcal{H}=0$ and take the z direction along $\mathbf{k}$. Because p_z has matrix elements only between states of the same m, the secular equation factors into a product of $2l_0+1$ factors, $D^{(0)}(\lambda,k^2)=\prod_{(m)}D_m(\lambda,k^2)$, where l_0 is the largest l value of the L. K. states used. From the invariance of the hamiltonian under reflection in a plane it follows that $D_m(\lambda,k^2)\equiv D_{-m}(\lambda,k^2)$ so that there is a double degeneracy at all $\mathbf{k}$ for $m\neq0$, and no degeneracy for $m=0$.

We shall now prove two properties of the secular determinant $D(\lambda,k_z',s,n)$ in the presence of $\mathcal{H}$, relating to its dependence on the set of quantum numbers m'; this dependence arises from the off-diagonal elements (5) and from the diagonal elements

$$(\Phi_{n-m'},\bar{k}^2\Phi_{n-m'})=k_z'^2+s(2n+1-2m'). \quad (7)$$

(1) By using the symmetry operation $y\rightarrow-y$ it is seen that the matrix elements of p_i between the $u_\mu(\mathbf{r})$ obey the relations

$$(p_z)_{l',m';\,l'',m'}=(p_z)_{l',-m';\,l'',-m'};\quad (p_\pm)_{l',m';\,l'',m''} =(p^\mp)_{l',-m';\,l'',-m''}. \quad (8)$$

From (5), (7), and (8) it follows that if the basic vectors $u_{t'l'm'}\Phi_{n-m'}$ are sent into $u_{t',l',-m'}\Phi_{n+m'}$ the matrix elements of the Hamiltonian undergo simply the transformation $\{m'\}\rightarrow\{-m'\}$. Since the determinant D is unchanged by this relabelling of rows and columns, it follows that D as a function of the set of numbers $\{m'\}$ is invariant under the operation of reflecting $\{m'\}$ into $\{-m'\}$. This is true only for $n\geqslant l_0$; for $n<l_0$ it is necessary to do the calculations individually for each n by deleting the rows and columns for which $n-m<0$.

(2) The second property to be proved is that D contains only even powers of each matrix element (5) (and of k_z') so that it is a polynomial in s, n, and m'. This property insures that the coefficients of the expansion in powers of s are finite for all n. To prove it we consider in a given term of D, the off-diagonal elements which connect m' with $m''=m'\pm1$ (m' is the row index, m'' the column index). The definition of a determinant implies that the two sets $\{m_i'\}$ and $\{m_i''\}$ must be identical. From $m''=m'\pm1$ it follows that always two factors with m' and m'' values interchanged occur together in each term of D. Hence D contains no square roots. A similar argument using the fact that the nonvanishing off-diagonal elements connect only states with values of l' differing by an odd number shows that only even powers of k_z' occur in D.

These two properties are the result of rotation-reflection invariance of our model. To obtain the secular equation we notice one more fact, that in the absence of $\mathcal{H}$ and taking instead of (4) a solution of definite k_x', the matrix elements for $m'=m''\pm1$ are obtained by substituting $k_x'^2$ for $2s[n+\frac{1}{2}-m'\pm\frac{1}{2}]$ in the matrix with the field present. By considering each term of D expanded in powers of $s(m'+m'')$ and using the symmetry of D under the transformation $\{m'\}\rightarrow\{-m'\}$ the secular equation is obtained to order s^2:

$$D(\lambda,k_z^2,n,s)=\prod\nolimits_m D_m[\lambda,k_z^2+s(2n+1)] +s^2G(\lambda,k_z^2,s(2n+1))+\cdots, \quad (9)$$

where G is a polynomial in its three arguments.

The solutions of (9) are of two types, depending on whether a branch of a band with $m=0$ or $|m|\neq0$ is under consideration:

(a) For $m=0$, the energy levels are

$$\lambda_{t,0}(k_z^2,n,s)=\lambda_{t,0}{}^{(0)}[k_z^2+s(2n+1)] +s^2\lambda_{t,0}{}^{(2)}(k_z^2,s(2n+1)), \quad (10)$$

where $\lambda_{t,0}{}^{(0)}(k^2)$ is the energy in the absence of $\mathcal{H}$ and

$$\lambda_{t,0}{}^{(2)}=-G(\lambda_{t,0'}{}^{(0)},k_z^2,s(2n+1))\Big/ \prod_{m'\neq0}{}' D_{m'}(\lambda_{t,0}{}^{(0)};k^2)\left(\frac{\partial D_0}{\partial\lambda}\right)_{\lambda=\lambda_{t,0}{}^{(0)}}. \quad (11)$$

(b) For $m\neq0$, $D_{|m|}$ occurs twice in (9) so that

$$\lambda_{t,|m|,\pm}(k_z^2,n,s)=\lambda_{t,m}{}^{(0)}\pm s\lambda_{t,|m|}{}^{(1)}+s^2\lambda_{t,|m|}{}^{(2)},$$

with

$$(\lambda_{t,|m|}{}^{(1)})^2=-G(\lambda_{t,m}{}^{(0)})\Big/ \prod_{m\neq'\pm m}{}' D_{m'}(\lambda_{t,m}{}^{(0)},k^2)\left[\left(\frac{\partial D_m}{\partial\lambda}\right)_{\lambda=\lambda_{t,m}{}^{(0)}}\right]^2 \quad (12)$$

and a more complicated expression for $\lambda_{t|m|}{}^{(2)}$. The linear terms $s\lambda^{(1)}$ correspond to the orbital moment arising from the double degeneracy in the absence of $\mathcal{H}$. Equation (12), and in case t is a degenerate band, Eq. (11) fail at $\mathbf{k}=0$ since the levels in the absence of $\mathcal{H}$ are $(2l+1)$ fold degenerate at that point and the denominators of (12) or (11) vanish. For degenerate bands, the magnetic levels in the vicinity of $\mathbf{k}=0$ must be considered individually. It is possible to prove, as a result of a further factorization of the secular equation for $k_z=0$, that at $k_z=0$, $\lambda_{t|m|}^{(1)}$ vanishes and the degeneracy of the nth levels belonging to the two branches t, $|m|$, $\pm$ is removed only to order s^2.

Remarks on the Energy Levels

(a) The first term $\lambda_{t,0}^{(0)}$ in (10) is identical with the result of the semiclassical quantization rule of Onsager[11] with a value of $\Theta=\frac{1}{2}$; this is seen by noticing that the area in k_x, k_y space embraced by the curve, intersection of a plane of constant k_z with the constant energy surface $\lambda_{t,0}^{(0)}(k^2)=\lambda_{t,0}^{(0)}(k_z^2,n,s)$ is equal to $2\pi s(n+\frac{1}{2})$. It is of interest to inquire whether there are cases in which the semiclassical treatment gives the complete answer. It can be shown, by using appropriate linear combinations of the basis functions, that if only s and p bands (in any number) are included, and in addition the interband elements of p_i are so large that the free mass terms $\bar{k}_i^2/2$ can be neglected, then $G\equiv 0$ so that $\lambda_{t,|m|}=\lambda_{t,m}^{(0)}$ for $m=0,\pm 1$. As soon as levels with $l>1$ are included, or when the free mass is not neglected, G does not vanish in general and level shifts occur.

(b) In the accompanying paper[7] the susceptibility resulting from the semiclassical quantization of the levels, i.e., for $\lambda_{t,0}=\lambda_{t,0}^{(0)}[k_z^2+s(2n+1)]$, is calculated as a part of the total χ and is denoted by χ_a. In view of some confusion which has occurred in the literature we want to stress that χ_a is not identical with the χ_3 term of Peierls[12] except for the case of free electrons.

The difference between the two is easy to see in the spherical approximation. The semiclassical levels are those of a Hamiltonian function $\lambda_{t,0}^{(0)}(\bar{k}_x^2+\bar{k}_y^2+k_z^2)$ where the dependence on the noncommuting operators $\bar{k}_x^2$, $\bar{k}_y^2$ is prescribed as follows: expand formally $\lambda_{t,0}^{(0)}(k_x^2+k_y^2+k_z^2)$ in powers of k_x^2, k_y^2, k_z^2, symmetrize each term with respect to k_x^2 and k_y^2 (e.g., write $k_x^2k_y^2+k_y^2k_x^2$ for $2k_x^2k_y^2$) and substitute the operators $\bar{k}_x^2$ and $\bar{k}_y^2$ for k_x^2 and k_y^2. The Hamiltonian for which the susceptibility is χ_3 is also obtained by symmetrization of $\lambda_{t,0}^{(0)}$ but the difference is that each term is symmetrized with respect to k_x and k_y (thus $k_x^2k_y^2$ is written as the sum of six terms). The levels of these two Hamiltonians differ by terms of order s^2 and hence lead to different susceptibilities.

EFFECT OF SPIN-ORBIT COUPLING

When spin-orbit coupling is included the treatment is similar to the foregoing, the difference being that: (a) the $u_{t,l,m}$ are replaced by spinors $u_{t,j,m}$ where $j=l\pm\frac{1}{2}$ is the total angular momentum with z component m, (b) the Zeeman energy $(g_s/2)\beta\mathcal{H}\sigma_z$ with $g_s=2.0023$ has to be added to the Hamiltonian, and (c) the velocity is now $\boldsymbol{\pi}=\mathbf{p}+(1/4c^2)\boldsymbol{\sigma}\times\boldsymbol{\nabla}V$, the σ_i being the Pauli matrices. The interband matrix elements of the Hamiltonian are due to $\pi_zk_z+\pi_-k_++\pi_+k_-$ where:

$$\pi_z=p_z+i\lambda(r)[(x-iy)\sigma_+-(x+iy)\sigma_-],$$

$$\pi_\pm=p_\pm\pm i\lambda(r)[(x\pm iy)\sigma_z-z\sigma_\pm],$$

with $\sigma_\pm=\sigma_x\pm i\sigma_y$ and $\lambda(r)=(1/8c^2)(1/r)(\partial V/\partial r)$. The matrix elements, $(\pi_z)_{\mu'\mu''}$, $(\pi_\pm)_{\mu'\mu''}$ do not vanish only for $m'=m''$, $m'=m''\pm 1$ as a consequence of the fact that the z component of angular momentum j_z commutes with π_z, $j_+\pi_-$, and $j_-\pi_+$. Therefore the components of the wave functions are of the type (4) but because m' is a half-integer, a half-integer must be added to the subscript of Φ. We shall associate the harmonic oscillator level n with $m'=-\frac{1}{2}$, so that in the expressions (5) and (7) for the matrix elements $n+\frac{1}{2}$ goes over into n. By using the symmetry operation JR, where J is the inversion of the space coordinates and R is a rotation by π around $0y$, the symmetry properties of the secular determinant can be found just as in the case of no spin-orbit coupling with the result that to order s^2, D is given by

$$D=\prod_m D_m(\lambda,\, k_z^2+2sn)+s^2G(\lambda,k_z^2,2ns). \tag{13}$$

Here the values of m range from $-(l_0+\frac{1}{2})$ to $+(l_0+\frac{1}{2})$, the $D_m(\lambda,k^2)$ are the factors of the secular equation in the absence of $\mathcal{H}$ with $D_m=D_{-m}$ and G is again a polynomial in its variables.

In spin resonance, the interaction $\sigma_\pm$ (transverse magnetic field) induces transitions between levels having the sets of harmonic oscillator quantum numbers, $\{n-m'-\frac{1}{2}\}$ associated with $u_{\mu'}$, differing by ± 1. When the levels thus connected belong to the two branches t, $|m|$, $\pm$ of the same band, (i.e., when they are Kramers-degenerate) the energy difference is proportional to s and defines the g factor, $g_{t,|m|}$. An expression for $g_{t,|m|}$ can be derived from (13) but it is not particularly illuminating and will be omitted.

USE OF PERTURBATION THEORY

The band structure of an actual crystal is in general not spherically symmetric; we shall outline in this section a perturbation treatment of the departure from sphericity and give the range of validity of such a treatment.

We write the crystal Hamiltonian matrix in the true L. K. states as the sum of a zero-order matrix H_0 having the structure of a spherically symmetric Hamiltonian and a perturbation matrix H'. The levels of H_0 are obtained as above. The elements of the matrix H' are constants or terms linear in the $\bar{k}_i$. Because of this property H' connects only a few eigenstates of the spherical Hamiltonian, having values of the harmonic

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[11] L. Onsager, Phil. Mag. **43**, 1006 (1952).

[12] R. Peierls, Z. Physik **80**, 763 (1933).

oscillator quantum numbers differing only by a small integer. These matrix elements, which are readily found, are of two types depending on whether they connect magnetic levels in different bands, or levels in the same band. The correction to the energy levels due to the former can be obtained by perturbation when the energy separation between the bands involved is large; this was done in reference 10. On the other hand, because the levels in one band are closely spaced in energy, the matrix elements of H' between these cannot be treated as perturbations on the individual levels. It has been shown by Peierls[12] that a perturbation expansion of the free energy is still possible in such cases.

The range of validity of a perturbation expansion in powers of H' has been found for the present case by using Peierls' argument[13] with a minor change because the unperturbed levels are discrete instead of continuous. Denoting by ζ the Fermi energy and by V the order of magnitude[14] of the matrix elements of H' between states in the band of interest, the requirement for the convergence of the expansion is that $V \ll kT$. However the condition for the convergence of the nonoscillatory part of the free energy, for $kT \ll \zeta$, is only that $V \ll \zeta$. This latter condition is equivalent to saying that the departure of the Fermi surface from a sphere must be small.

SUMMARY

We have shown in this paper that the energy levels of an electron in a periodic potential and a magnetic field can be obtained rather simply if one makes the spherical approximation to the band structure. General expressions for the expansions of the levels in powers of the magnetic field have been given. Spin-orbit coupling has been included so that it is possible to obtain the g factor for spin resonance as function of position in the band. Finally, for substances with nearly spherical energy bands, these levels can be conveniently used for a calculation of the nonoscillatory part of the free energy from which magnetic properties such as the susceptibility can be calculated.

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I wish to thank E. I. Blount, R. Bowers, and T. Kjeldaas for useful comments on this work.

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[13] The reader is referred to reference 12, pp. 772–774 for the detailed argument.

[14] The quantity V is at most of order $|H'|$; it may be smaller than this if the bands that are split by the symmetry of the crystal are far removed from the band which contains the electrons.

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Further Experiments on the Sidewise Motion of 180° Domain Walls in $BaTiO_3$

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Techniques have been developed to extend the measured electric field dependence of the sidewise 180° domain-wall velocity in liquid-electroded $BaTiO_3$ crystals. The wall velocity data now cover about eight decades of velocity. The wall velocity is given by $v_\infty \exp(-\delta/E)$, where δ is found to increase slightly with field. The temperature dependence of v has been measured over a limited temperature range and the data show that δ varies with temperature faster than T^{-1}. The shapes and orientations of the reversed domains are field dependent. As the electric field is increased, the approximately square reversed domains observed in the low-field region go over into octagonal domains. At still higher fields, approximately square domains rotated by 45° about the ferroelectric axis with respect to the low-field domains are observed. Several of the important features of the sidewise wall motion are consistent with a nucleation-controlled model which is currently under investigation.

INTRODUCTION

In a recent paper,[1] the electric field dependence of the sidewise 180° domain-wall velocity in liquid-electroded $BaTiO_3$ crystals has been described. The experiments involved electrical measurements of the rate of growth of a single reversed domain as a function of the applied electric field. The experimental techniques were such that the wall velocity could not be obtained for fields higher than about 350 v cm^{-1}. In the present research, methods are employed which permit one to extend the earlier measurements of the sidewise 180° domain-wall velocity, and other relevant data, to fields of the order of a thousand volts per centimeter. The earlier data will be referred to as low-field data while the present data will be termed high-field data. The temperature dependence of the wall velocity, which preliminary data[1] indicated was quite pronounced, has been investigated in more detail. Square reversed domains with sides at approximately 45° to the crystalline a axes have been observed[1,2] in the low-field region.

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[1] R. C. Miller and A. Savage, Phys. Rev. **112**, 755 (1958).

[2] R. C. Miller, Phys. Rev. **111**, 736 (1958).