the quadrupole coupling data so that the molecular orbitals for these cases are expected to be correct. Also, the tetrahedral case of YIG has been taken instead of the octahedral case since the experimental data of the isomer shifts in YIG (tet) and Fe_2O_3 are not as close as in YIG (oct) and Fe_2O_3; consequently, the error introduced in the calculation will be smaller. Thus, using $\delta(Fe_2O_3) = 0.047$ [4] and δ(YIG (tet)) $= 0.032$ [10] (in units of cm/sec) and the corresponding calculated $\rho_a'(0)$ from Table I, one gets $K_0 = -0.01496 a_0^{-3}$ cm/sec and $C = -14.649 a_0^{-3}$.

Knowing K_0 and C one next calculates δ for all the other cases from the calculated $\rho_a'(0)$ (Table I). The values of δ so obtained are also listed in Table I together with the experimental results[4,12] for the cases under consideration. The errors in the calculated values of δ have arisen from the uncertainties in the crystal-structure data as regards the ligand distances a_g which are required for the evaluation of the overlap integrals and the ligand functions [see Eq. (4)]. It should be noted that the calculated δ for YIG (oct) gives perfect agreement with the experimental results which proves the consistency of the method. The calculated values of δ in other cases also agree perfectly with the experimental data (see Table I) within the experimental errors except for GdIG (tet) where the deviation is rather large.

From the deduced value of K_0 it is important to extract information regarding the relative change in the charge radius, $\delta R/R$, of the Fe^{57} nucleus. Using $S'(Z) = 1.29$,[5] $R = 1.2A^{1/3}$ F (A being the atomic number), one obtains $\delta R/R = -4.11 \times 10^{-4}$, a result close to the value[13] -4×10^{-4} obtained by Simanek and Wong[14] from the pressure dependence of the isomer shift in $KFeF_3$ and the value[13] -3.9×10^{-4} as suggested by Goldanskii.[15] For the sake of comparison we also give the result[13] $\delta R/R = -1.4 \times 10^{-3}$ as derived by Walker, Wertheim, and Jaccarino.[4]

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Linear Magnetoresistance and Anisotropic Quantum Fluctuations

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We propose a theory which accounts for the linear magnetoresistance found in the transverse and longitudinal components in various metals. The theory is based on the existence of quasiperiodic static fluctuations, which have the anisotropy of the lattice and may be due to electron-phonon and/or electron-electron interactions. The fluctuations produce no noticeable change in the static properties of the metal but produce the dominant linear increase of the resistance at high magnetic fields.

The phenomenon of linear magnetoresistance has been in the literature for many years.[1] It has been found in several metals (e.g., aluminum, indium, the alkali metals) of which potassium can be considered the clearest example.[2] The linear increase of the transverse and longitudinal resistances, as the magnetic field strength H increases, seems to violate the general behavior of the magnetoresistivity tensor in the limit $H \to \infty$, $\omega_c \tau \gg 1$, as predicted by Lifschitz

and his collaborators[3] and as verified experimentally for most metals.[4]

The general features of the experiments can be summarized as follows: (i) The effect appears in those metals with no open orbits and such that as $H \to \infty$, the Lifschitz theory predicts a saturating behavior; (ii) the linear behavior is found for many experimental geometries and for various methods of measuring the resistance; (iii) it appears for the longitudinal and transverse components of the resistivity tensor; (iv) the linear behavior is present for magnetic fields between approximately 5 and 110 kG (this is equivalent to $\omega_c\tau$ varying typically between 10 and 350); (v) even at the higher fields at which the experiments have been performed ($\gtrsim$ 100 kG) the linear increase continues unchanged with no tendency to saturation or any other departure from linearity; (vi) the dimensionless slope

$$S \equiv \frac{\Delta\rho/\rho_0}{\omega_c\tau} \tag{1}$$

is characteristically a small number of the order of 10^{-4} to 10^{-2}; (vii) the slope S seems to be quite sensitive to sample preparation and handling, especially to strains.

Several theoretical explanations for the phenomenon have been put forward. They are in general of two kinds: morphological or intrinsic. The morphological (geometrical) explanations are based essentially on the geometry of a given experiment, the linear term in the magnetoresistance arising from specific boundary conditions in the solution of Maxwell's equations[5,6] or from discontinuities or macroscopic variations of some constitutive parameters such as local density of electrons, crystallite orientation, etc. The fact that the linear behavior is found in *all* samples—regardless of shape, contacts, and quality—makes all these explanations rather implausible. In addition, the observation of the linear term as predicted by most of these theories depends on the fulfillment of experimental conditions (geometry of the leads, values of the magnetic field, etc.) which are not realized in practice.[5]

The intrinsic theories are of two subclasses: structural or transport. Structural theories assume that the metals for which linear magnetoresistance is observed are not *normal* metals in the usual sense: They have either strong spin correlations[7] which effectively produce a double periodicity in the lattice and the appearance of lattice-related energy gaps, or they are metals whose ground state is defined by a spin-density wave or a charge-density wave.[8] In this last case energy gaps also appear but they are essentially attached to the electronic Fermi surface and are therefore in general incommensurable with the lattice periodicity. The drawback of these theories is that they give a change in equilibrium properties which should be observable in other experiments, e.g., the de Haas–van Alphen effect. Such is definitely not the case.[9]

The intrinsic transport theories propose various kinds of scattering mechanisms which cannot be incorporated in a relaxation-time approximation. One such theory,[10] the so-called "hot-spot" model, requires strong scattering probabilities between well-defined "spots" on opposite sides of the Fermi surface. If the scattering rate on the "hot spots" is given by $1/T$, and the normal relaxation time in the rest of the Fermi surface is given by τ, then in the region $\omega_c\tau \gg 1, \omega_c T \ll 1$, the resistivity tensor exhibits a linear behavior such that S, given by (1), takes the form

$$S \cong K\nu Q(1-Q)[1-2(1-Q)Q]^{-1}, \tag{2}$$

where K is a numerical constant of the order of 1 which depends on the geometry of the Fermi surface, ν is the fraction of electrons participating in "hot-spot" scattering (i.e., proportional to the area of the "hot spots"), and Q is the probability that an electron traveling on the Fermi surface under the influence of the magnetic field and entering a given "hot spot" emerges at the opposite side of the Fermi surface. In order to have a constant, magnetic-field–independent S, Q should be also magnetic field independent. Young[10] proved that this is so only for $\omega_c T \ll 1$, in which case $Q \cong 0.5$. Since S is experimentally a very small quantity and constant up to very high fields, this theory can only explain the experimental results if the hot spots are extremely small ($\nu \ll 1$) and extremely hot ($\omega_c T \ll 1$ for say 100 kG) which is physically unreasonable.

We would like to propose here a new mechanism which can yield a linear magnetoresistance and be consistent with the experimental facts (i) to (vii) mentioned above. It is an intrinsic transport mechanism which can be easily connected to Young's hot-spot theory. From a pragmatic point of view, the most serious problem in Young's approach is that the solution of Boltzmann's equation with localized scattering cannot give at $\omega_c T \ll 1$ a value of Q different from $\frac{1}{2}$, and there is no range in magnetic field other than

$\omega_c T \ll 1$ for which Q is essentially constant, i.e., magnetic field independent.

If the problem is now faced not as a transport scattering problem, but rather as a quantum-mechanical tunneling problem, a completely different result emerges. For an electron (mass m, charge $-e$) moving in a constant magnetic field parallel to the z axis and under the influence of a quasiperiodic potential $V(x)$ of wave vector $\vec{g} = (g, 0, 0)$,

$$V(x) = \tfrac{1}{2} D(x - x_0)(V_g e^{igx} + V_g^* e^{-igx}), \tag{3}$$

where $D(x - x_0)$ is an envelope function $[D(0) = 1]$ chosen to be of the form

$$D(x) = \exp[-\eta^2 x^2/4] \tag{4}$$

and centered about an arbitrary point x_0, a straightforward calculation, following Pippard,[11] yields for the maximum probability of transition Q from $\vec{k}$ to $\vec{k}+\vec{g}$ across the Fermi surface ($|\vec{k}| = |\vec{k}+\vec{g}| = k_F$),

$$Q = (Q_0^{-2} + H^2/H_0^2)^{-1/2}, \tag{5}$$

where

$$H_0 \equiv \tfrac{1}{4}\pi m^2 c |V_g|^2 / e\hbar^3 |k_x k_y|, \tag{6}$$

$$Q_0 \equiv (\pi^{1/2} |V_g| m/\hbar^2 \eta |k_x|)^2. \tag{7}$$

Formula (5) is valid if $Q \ll 1$. It can be easily recognized that H_0 given by (6) is the usual magnetic breakdown parameter,[11,12] which for typical periodic potentials of a lattice takes values from 10^3 to 10^6 G. According to (5) the tunneling probability Q is a constant equal to Q_0 for values of field $H < H_0/Q_0$, and it takes the usual magnetic breakdown form[13]

$$Q \cong H_0/H$$

for $H \gg H_0/Q_0$. If we take the conservative values $Q_0 = 0.01$ and $H_0 = 10^4$ G, Q is a small constant quantity Q_0 up to values of $H \cong 10^6$ G. This would yield a linear magnetoresistance with a slope of order νQ_0 for values of H up to about a million gauss, and a change to saturation from there onwards. Even if $\nu = 1$, the small-slope linear magnetoresistance can be obtained. It is therefore not necessary to have small "hot spots" and extremely strong scattering to satisfy the conditions found experimentally.

Two points are worth emphasizing: (a) The results (5)–(7) are essentially independent of the particular choice of the envelope function (4); Q_0 as given by (7) can in general be interpreted in terms of the value at the origin of the Fourier transform of $D(x)$. (b) The results (5)–(7) are only functions of $|V_g|$, i.e., independent of the phase of V_g. We can now think of a statistically fluctuating potential such that the ensemble average $\langle V_g \rangle$ is zero but such that $\langle V_g V_g^* \rangle \neq 0$. Such a fluctuating potential would yield the same results (5)–(7).

Although we have shown explicitly the case of a scattering quasiperiodic potential, it can be inferred that the same effect should arise from static quantum-mechanical fluctuations in the ground state of the electron gas in the crystal. Such fluctuations, in order to explain the linear magnetoresistance, should be (A) anisotropic over the Fermi surface and (B) coherent over a length $\sim 1/\eta$ in space and such that $\eta < g$.

The origin of such coherent, anisotropic quantum-mechanical fluctuations could be (I) electron-phonon interactions; (II) electron-electron interactions.

In case (I) the virtual emission and absorption of a phonon and the zero-point vibration in the phonon modes can easily provide the kind of effect we are expecting here, in which the virtual umklapp contribution yields the expected quantum "hot spots" for those regions of the Fermi surface which approach the Brillouin zone boundary.

In the case II, the lattice potential (or the true Bloch states) should be accurately taken into account, since the anisotropy in the electron-electron interaction (the only part that contributes to the magnetoresistivity) can only appear through the influence of the lattice.

Either case looks like a suitable candidate to explain quantitatively the experimental results: Both mechanisms are strongly strain dependent and they yield, in principle, values of similar order of magnitude. For the parameters of potassium ($k_F = 0.73$ Å^{-1}, $\epsilon_F = 2.1$ eV) and with $|V_g| \sim 0.01$ eV and $1/\eta \sim 20$ Å, we obtain $Q_0 \sim 10^{-2}$ and $H_0 \sim 10^4$ G. This corresponds to fluctuations over 5 to 10 lattice sites with values of the anisotropic component of the fluctuating potential at its maximum of about $\frac{1}{200}$ of the Fermi energy and $\frac{1}{20}$ of the value of the (110) Fourier component of the lattice potential.[9]

Finally, since the proposed mechanism transfers electrons back and forth between regions of the Fermi surface which are widely separated, it does contribute equally to a linear increase in longitudinal[14] and transverse components of the magnetoresistivity tensor. It does not change appreciably the energy spectrum of the electron

quasiparticles[15] and, except for the usual Dingle contribution to the amplitude, it does not change the de Haas–van Alphen spectrum.

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$$Q(H=0)=\tanh^2(Q_0^{1/2}), \quad Q=1-\exp(-1/R^{1/2}),$$

$$R\equiv\frac{H^2}{H_0^2}+\frac{1}{4\ln^2[\cosh(Q_0^{1/2})]},$$

which reduce to the usual breakdown formula of Ref. 12 as $\eta\to 0$ and $Q_0\to\infty$, $Q=1-\exp(-H_0/H)$. We have obtained similar results for nonlinear electric field effects and the consequent Zener breakdown.

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Magnetic Metal-Nonmetal Transitions: A Simple Model

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A two-band model of a solid is presented which exhibits simultaneous first-order metal-nonmental and antiferromagnetic phase transitions in the Hartree-Fock approximation.

As originally envisioned by Mott, a first-order metal-nonmetal (MNM) transition should occur with changes in the interatomic distances.[1,2] A surprisingly large number of transition-metal and rare-earth compounds exhibit some type of MNM transition. These transitions are generally observed with changing temperature rather than changing pressure, and it is not yet clear that these transitions are true Mott transitions. A large number of these MNM compounds have two types of electronic states (e.g., s-p or d bands for the transition-metal chalcogenides) which can participate in the conduction process. It is our opinion that the existence of the two types of electronic states is of basic importance and should not be ignored.

Several MNM transitions (e.g., the transitions in NiS and V_2O_3) are accompanied by a first-order antiferromagnetic transition.[1] It has been suggested that this type of transition can be explained in terms of a large-amplitude spin density wave (SDW).[3] If the energy gaps resulting from the antiferromagnetic SDW's are large enough, an insulating antiferromagnet will result. However, a MNM transition will occur at the Néel temperature only if the magnetic order disappears suddenly, and simple SDW theory predicts a second-order Néel transition. Furthermore, the validity of the SDW approach is not clear for interaction strengths large enough to produce an insulating magnetic state.

As an alternative to SDW theory, we consider