mode cannot contribute significantly to the thermal conductivity. The reason for this probably lies in the magnitude of the group velocity. Unpublished calculations show that at about 20°K, the out-of-plane group velocity is smaller than the softest in-plane mode by a factor of at least 13. This in-plane mode has a constant group velocity, a T^2 specific heat contribution down to very low temperatures and a Debye temperature of about 1600°K. If this mode is the major contributor to the thermal conductivity, the values of the crystallite sizes obtained in the present paper would be wrong by about 50%, which would change none of the conclusions.

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Longitudinal Magnetoresistance in the Quantum Limit

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A study has been made of the effect of a magnetic field on the scattering of electrons in a semiconductor with spherical energy surfaces. The theory has been applied to longitudinal magnetoresistance in the case of a very large magnetic field and low temperatures so that all conduction electrons are in the ground oscillator state. Relaxation times for phonon and ionized impurity scattering have been calculated and the corresponding mobilities for a degenerate and nondegenerate semiconductor have been derived. Contrary to the zero magnetoresistance predicted by the usual Boltzmann theory, a field-dependent magnetoresistance is found. For a nondegenerate semiconductor and in the ionized impurity scattering range a negative magnetoresistance is predicted.

I. INTRODUCTION

THE electrical resistivity of a wire is usually affected somewhat by the presence in the wire of a magnetic field. This magnetoresistance may be large or small, and it depends on the nature of the energy band structure of the material, the carrier mobilities, the strength of the magnetic field, and the temperature.

Theories of magnetoresistance are usually based on the one electron band model of solids, and, ordinarily, on a Boltzmann theory treatment of transport. Such theories with various degrees of generality have been given by many authors.[1]

We will concern ourselves here with the result, valid for the most general energy surface and Boltzmann scattering integrals, that for sufficiently high values of a magnetic field the resistance of a wire approaches a limiting value independent of the strength of the magnetic field. The predicted saturation of the magnetoresistance is a consequence of the assumption in most theories that the scattering processes are not much affected by the presence of a magnetic field. This assumption is valid for magnetic fields

$$H \ll mc/e\tau, \tag{1.1}$$

in which m is the carrier effective mass and τ is the mean free time. This condition may also be written as

$$\omega_0\tau \ll 1, \tag{1.2}$$

in which ω_0 is the cyclotron resonance angular frequency which is directly proportional to the magnetic field.

On an intuitive basis we might expect that for magnetic fields such that $\omega_0\tau > 1$, the relaxation time may become appreciably dependent on the strength of the magnetic field. For in so strong a magnetic field, the path of the carrier between collisions is very much curved since the period of execution of a complete circular orbit is less than the time between collisions. Thus for $\omega_0\tau \gtrsim 1$, the predictions of the ordinary Boltzmann treatment, which assumes the collisions unaffected by the magnetic field, cannot be trusted without closer examination.

Treatments of electric conduction in strong magnetic fields have been made by Titeica[2] and Davydov and Pomeranchuk.[3] Each of these treatments was somewhat special, but both showed that in magnetic fields for which $\omega_0\tau \gg 1$ there can be noteworthy effects on the magnetoresistance arising from the quantization of the electron orbits. It is such effects that we wish to discuss in the following work.

The theory of Titeica concerned the resistivity of a good metal in which the chief mechanism of scattering

[1] J. McClure, Phys. Rev. **101**, 1642 (1956). This reference contains references to other relevant work.

[2] V. S. Titeica, Ann. Physik **22**, 129 (1935).

[3] B. Davydov and I. Pomeranchuk, J. Phys. (U.S.S.R.) **2**, 147 (1940).

is the electron lattice interaction. Thus in this theory it is assumed that the electron gas is degenerate and that the electron phonon interaction diminishes strongly below the Debye temperature. The aim of the theory was to explain certain results of Kapitza of the magnetoresistance of metals in fields up to several hundred thousand gauss.

The theory of Davydov and Pomeranchuk concerned the resistivity of a semimetal in which the chief mechanism of scattering is the interaction of electrons with very strongly localized imperfections. Thus in this theory the electron gas is assumed degenerate or nearly so, and the scattering interaction is temperature independent and can be represented by a set of delta functions in space. The aim of the theory was to explain certain features of the strong-field magnetoresistance of bismuth in the temperature interval for which impurity scattering is dominant.

In the following, we present a theory of the magnetoresistance of a semiconductor or semimetal interacting either with phonons or ionized impurities. In our theory the Fermi energy will be assumed very small, so the electron-phonon interaction will remain strong for temperatures far below the Debye temperature. The electron gas may be either degenerate or nondegenerate. We will be concerned primarily with the conductivity of carriers under conditions such that

$$\hbar\omega_0 > \epsilon \tag{1.3}$$

in which ϵ is the energy of the carrier.

We will limit our attention to the case that the magnetic field is parallel to the applied electric field. We do this for two reasons. One is that the treatment of the transverse problem is somewhat more complicated and presents points which we don't wish to discuss in this paper. The other is that quantum effects on the longitudinal magnetoresistance are somewhat more clear cut, since in the simple case we will discuss, the usual Boltzmann theory predicts no longitudinal magnetoresistance at all.

In the theory presented here, a single simple energy band with isotropic effective mass is assumed. This assumption could be generalized somewhat in that an ellipsoidal energy surface could be assumed, but for a variety of reasons we think it best to present here only the simplest case.

The general idea of our treatment is to make a transport theory using the eigenstates of the carrier in the magnetic field. Calculation of the scattering integral in these states takes properly into account the effect of the magnetic field on the scattering processes. Since we shall be concerned only with the case that $\hbar\omega_0 > \epsilon$, i.e., all carriers are in the lowest quantum state of the transverse motion in the magnetic field, we speak of "magnetoresistance in the quantum limit."

Our calculation is conveniently broken into several parts. In the first we calculate the energy eigenstates which are required for the strong-field transport problem and the transition matrix elements between these states. Next we calculate the momentum transfer relaxation times for lattice and impurity scattering. Finally, we calculate the conductivities on various assumptions about temperature and degree of degeneracy.

II. WAVE FUNCTIONS AND TRANSITION MATRIX ELEMENTS

We consider a one electron problem for which the Hamiltonian (for a magnetic field H along the z axis) is

$$\mathcal{H}=\frac{1}{2m}[p_x^2+(p_y+m\omega_0 x)^2+p_z^2]. \tag{2.1}$$

We have used the gauge which is particularly suited to the discussion of electrical conductivity.[2] The eigenvalues and eigenfunctions are

$$\epsilon(Nk_yk_z)=\hbar\omega_0(N+\tfrac{1}{2})+\hbar^2k_z^2/2m, \tag{2.2}$$

$$\psi(Nk_yk_z)=\varphi_N(x+\lambda^2k_y)e^{ik_yy}e^{ik_zz}L_y^{-\frac{1}{2}}L_z^{-\frac{1}{2}}. \tag{2.3}$$

Here k_y and k_z are the wave numbers associated with the y and z coordinates and L_y, L_z are the corresponding normalization lengths. $\varphi_N(x+\lambda^2k_y)$ is the wave function for a harmonic oscillator of frequency ω_0 in its Nth excited state and oscillating about the point

$$-\lambda^2k_y=-\hbar k_y/m\omega_0. \tag{2.4}$$

We shall be concerned only with the ground oscillator state for which

$$\varphi_0(x+\lambda^2k_y)=(\pi\lambda^2)^{-\frac{1}{4}}\exp\left[-\frac{1}{2}\left(\frac{x+\lambda^2k_y}{\lambda}\right)^2\right] \tag{2.5}$$

and

$$\epsilon(0k_yk_z)=\tfrac{1}{2}\hbar\omega_0+\epsilon_z, \tag{2.6}$$

with $\epsilon_z=\hbar^2k_z^2/2m$, the kinetic energy of the electron in the z direction.

Each of the wave functions $\psi(Nk_yk_z)$ describes a state for which the electron probability distribution is different from zero only in a slab symmetrically disposed about the plane $x=-\lambda^2k_y$.

A calculation of the electric current carried by an electron in one of these states shows that the average electric current is in the z direction and is given by

$$J(Nk_yk_z)=(-e)\hbar k_z/m. \tag{2.7}$$

The mean values of the operators for the components of electric current in the x and y directions, *viz.*, $J_x=(-e/m)p_x$ and $J_y=(-e/m)(p_y+m\omega_0x)$, vanish for each of the energy states, regardless of the values of k_y and N.

We will calculate next the transition matrix element of the function $e^{i\mathbf{q}\cdot\mathbf{r}}$ between two energy states. In most of this work we will be concerned with magnetic fields

so large that the available thermal energy is insufficient to raise the electron to an excited oscillator state. In that case the appropriate matrix element is

$$\langle 0k_y'k_z'|e^{i\mathbf{q}\cdot\mathbf{r}}|k_zk_y0\rangle=\delta(k_y'-k_y-q_y)\delta(k_z'-k_z-q_z)\times\exp\{-\tfrac{1}{4}\lambda^2[q_x^2+q_y^2+2iq_x(k_y'+k_y)]\}. \quad (2.8)$$

From Eq. (2.8) it will follow that the transition probabilities which we will need will be proportional to $\exp[-\frac{1}{2}(q_x^2+q_y^2)\lambda^2]$.

III. RELAXATION TIME FOR ACOUSTICAL SCATTERING

We now wish to calculate the relaxation time for momentum transfer for electron in a definite energy state $\psi(Nk_yk_z)$ due to collisions with acoustical lattice vibrations. We will consider only the case $N=0$, $\Delta N=0$, i.e., the electron is executing zero-point motion transverse to the magnetic field both before and after the scattering.

The perturbation Hamiltonian can be written

$$H_1=E_1\textstyle\sum_{\mathbf{q}} qQ_{\mathbf{q}}e^{i\mathbf{q}\cdot\mathbf{r}}. \quad (3.1)$$

The scattering rate into unit volume of $\mathbf{q}$ space will be taken from perturbation theory. What we will calculate, however, is not the scattering rate but the rate of loss of momentum in the z direction. We can write

$$\dot{k}_z=\sum_{k_y'k_z'} W(k_yk_z,k_y'k_z')(k_z'-k_z). \quad (3.2)$$

Now, for acoustic lattice vibrations with $\omega(\mathbf{q})=sq$, where ω is angular frequency, $\mathbf{q}$ the wave vector of the normal modes of vibrations of the lattice, and s the sound velocity, the transition probability per unit time is

$$W(\alpha,\alpha')=\frac{\pi}{V}\left(\frac{E_1^2}{\rho s}\right)\sum_{\mathbf{q}}[|\langle\alpha'|e^{i\mathbf{q}\cdot\mathbf{r}}|\alpha\rangle|^2q(N_{\mathbf{q}}+1)\times\delta(\epsilon_{\alpha'}-\epsilon_\alpha+\hbar\omega)+|\langle\alpha'|e^{i\mathbf{q}\cdot\mathbf{r}}|\alpha\rangle|^2\times qN_{\mathbf{q}}\delta(\epsilon_{\alpha'}-\epsilon_\alpha-\hbar\omega)]. \quad (3.3)$$

Here, α denotes the pair of quantum numbers k_y, and k_z, α' denotes the pair k_y' and k_z', V is the volume, and ρ the mass density of the specimen. $N_{\mathbf{q}}$ is the number of phonons $\mathbf{q}$.

We will be concerned here with the case that the electron energy is very small, $\epsilon_\alpha\sim kT$. Then for temperatures $T\gtrsim 1°\mathrm{K}$, the energy $\hbar\omega(\mathbf{q})$ of the phonons absorbed or emitted is much smaller than that of most of the electrons, i.e., $\hbar\omega\ll\epsilon_\alpha\sim kT$. We can then take the collisions as elastic and the distribution of the concerned phonons as classical, i.e., $N_{\mathbf{q}}\cong N_{\mathbf{q}}+1\cong kT/\hbar\omega=kT/\hbar qs$. Combining absorption and emission, we thus have

$$W(\alpha,\alpha')=A\delta(\epsilon_{\alpha'}-\epsilon_\alpha)\frac{1}{V}\sum_{\mathbf{q}}|\langle\alpha'|e^{i\mathbf{q}\cdot\mathbf{r}}|\alpha\rangle|^2, \quad (3.4)$$

where

$$A=(2\pi/\hbar)(E_1^2kT/\rho s^2). \quad (3.5)$$

Using Eq. (2.8) for the matrix element, we find

$$W(k_yk_z,k_y'k_z')=A\delta(\epsilon_z'-\epsilon_z)\frac{1}{V}\times\exp[-\tfrac{1}{2}\lambda^2(k_y'-k_y)^2]\sum_{q_x}\exp(-\tfrac{1}{2}\lambda^2q_x^2).$$

It is instructive to calculate the transition probability to all states with given k_z',

$$W(k_z,k_z')=\sum_{k_y'}W(k_yk_z,k_y'k_z');$$

we find

$$W(k_z,k_z')=A\delta(\epsilon_z'-\epsilon_z)\frac{2\pi}{L_z}N(k_z'), \quad (3.6)$$

where

$$N(k_z')=\frac{1}{(2\pi)^2}\frac{1}{\lambda^2}=\frac{1}{(2\pi)^2}\frac{m}{\hbar^2}\hbar\omega_0 \quad (3.7)$$

is the density of states (not including spin) per unit wave number interval [see Eq. (5.3)]. This demonstrates that backward and forward scattering (the only two possibilities) are equal, in exact analogy to the isotropic scattering of the field-free case. The difference between the two cases is twofold: the magnetic field, in the quantum limit, makes the motion of the carrier one dimensional and alters the density of states.

Defining the relaxation time ${\tau_H}^L$ by $1/{\tau_H}^L=-\dot{k}_z/k_z$, we get from Eqs. (3.2) and (3.6)

$$\frac{1}{{\tau_H}^L}=\sum_{k_z'}W(k_z,k_z'), \quad (3.8)$$

which yields

$$\frac{1}{{\tau_H}^L(\epsilon_z)}=A\int\delta(\epsilon_z'-\epsilon_z)N(\epsilon_z')d\epsilon_z'=AN(\epsilon_z), \quad (3.9)$$

where now

$$N(\epsilon_z)=\frac{1}{(2\pi)^2}\frac{1}{2}\left(\frac{2m}{\hbar^2}\right)^{\frac{3}{2}}\hbar\omega_0\epsilon_z^{-\frac{1}{2}} \quad (3.10)$$

is the density of states with energy ϵ_z per unit energy interval (spin not included). We thus see that the effect of the magnetic field on the lattice relaxation time is directly given by its effect on the density of states.

The corresponding relaxation time in the absence of the magnetic field is found with a similar analysis. In this case the matrix element $\langle\alpha'|e^{i\mathbf{q}\cdot\mathbf{r}}|\alpha\rangle=\delta(\mathbf{k}'-\mathbf{q}-\mathbf{k})$, and thus

$$W(\mathbf{k},\mathbf{k}')=(A/V)\delta(\epsilon_{\mathbf{k}'}-\epsilon_{\mathbf{k}}).$$

As before

$$\frac{1}{{\tau_0}^L(\epsilon)}=\sum_{\mathbf{k}'}W(\mathbf{k},\mathbf{k}')=AN_0(\epsilon_{\mathbf{k}}), \quad (3.11)$$

where now

$$N_0(\epsilon)=\frac{1}{(2\pi)^2}\left(\frac{2m}{\hbar^2}\right)^{\frac{3}{2}}\epsilon^{\frac{1}{2}} \tag{3.12}$$

is the density of states (not including spin) in the absence of the magnetic field, and $\epsilon_k=\hbar^2k^2/2m$ is the kinetic energy of the electron.

Combining (3.9) and (3.11), we get

$$\frac{\tau_H{}^L}{\tau_0{}^L}=\frac{N_0(\epsilon)}{N(\epsilon_z)}=\frac{\epsilon^{\frac{1}{2}}\epsilon_z{}^{\frac{1}{2}}}{(\hbar\omega_0/2)}. \tag{3.13}$$

Equation (3.13) shows that for electrons of kinetic energy less than $\hbar\omega_0/2$ the relaxation time is always smaller in the quantum limit than in zero field.

IV. RELAXATION TIME FOR IONIZED IMPURITY SCATTERING

We will treat ionized impurity scattering using a screened Coulomb potential of a single ionized impurity,

$$v(\mathbf{r})=\pm(e^2/\kappa)(e^{-r/r_s}/r). \tag{4.1}$$

In the Appendix we prove that this is the self-consistent potential energy of an electron around a charged impurity, under a simplifying assumption about the reaction of the free electrons to the extra charge. In Eq. (4.1), κ is the dielectric constant and r_s the appropriate screening length, expressions for which are derived in the appendix for different conditions of interest.

In the second order of perturbation theory we may neglect any effects due to coherence of the scattering amplitudes from different scattering centers. Thus we find for the transition rate per unit time due to interaction with ionized impurities

$$W(k_yk_z,k_y'k_z')$$

$$=\frac{2\pi}{\hbar}\sum_{\mathbf{R}}|\langle 0k_y'k_z'|v(\mathbf{r}-\mathbf{R})|0k_yk_z\rangle|^2\delta(\epsilon_z'-\epsilon_z). \tag{4.2}$$

In Eq. (4.2), $\mathbf{R}$ denotes the position of an impurity in the lattice. Writing

$$v(\mathbf{r}-\mathbf{R})=\pm\frac{4\pi e^2}{\kappa}\frac{1}{V}\sum_{\mathbf{q}}\frac{e^{i\mathbf{q}\cdot(\mathbf{r}-\mathbf{R})}}{q^2+1/r_s{}^2},$$

we can evaluate the matrix elements by making use of the integral given in Eq. (2.8). Thus, for a random distribution of impurities,

$$\sum_{\mathbf{R}}|\langle 0k_y'k_z'|v(\mathbf{r}-\mathbf{R})|0k_yk_z\rangle|^2=\left(\frac{4\pi e^2}{\kappa}\right)^2\frac{N_I}{V}$$

$$\times\sum_{q_x}\frac{\exp\{-\frac{1}{2}\lambda^2[q_x{}^2+(k_y'-k_y)^2]\}}{[q_x{}^2+(k_y'-k_y)^2+(k_z'-k_z)^2+1/r_s{}^2]^2}, \tag{4.3}$$

where N_I=concentration of ionized impurities.

If we calculate the backward and forward scattering probability we see that the former is smaller than the latter, in contrast to the case of phonon scattering. Only the backward scattering contributes to the relaxation of momentum.

We obtain after some calculations

$$\frac{1}{\tau_H{}^I}=\frac{\pi e^4N_I}{\kappa^2(2m)^{\frac{1}{2}}}\epsilon_z{}^{-\frac{3}{2}}\frac{I(\gamma)}{1+(\epsilon_s/4\epsilon_z)}, \tag{4.4}$$

where

$$\epsilon_s=\frac{\hbar^2}{2m}\frac{1}{r_s{}^2},\quad \gamma=\frac{\epsilon_s}{\hbar\omega_0}\left(1+4\frac{\epsilon_z}{\epsilon_s}\right), \tag{4.5}$$

and

$$I(\gamma)=\int_0^\infty xe^{-x}dx/(x+\gamma)=1+\gamma e^\gamma\,\mathrm{Ei}(-\gamma), \tag{4.6}$$

$\mathrm{Ei}(-\gamma)$ being the exponential integral. In the range of interest, i.e., $0\lesssim\gamma\lesssim10$, this can be approximated

$$I(\gamma)\cong1/(1+\gamma). \tag{4.7}$$

In the absence of the magnetic field, a similar analysis yields the following expression for the ionized impurity relaxation time

$$\frac{1}{\tau_0{}^I}=\frac{\pi e^4N_I}{\kappa^2(2m)^{\frac{1}{2}}}\epsilon^{-\frac{3}{2}}[\ln(1+\beta)-\beta/(1+\beta)], \tag{4.8}$$

where $\beta=4\epsilon/\epsilon_s$.

We observe that the factor $I(\gamma)/[1+(\epsilon_s/4\epsilon)]$ in Eq. (4.4) remains always between 0 and 1 for increasing values of ϵ_z, whereas the factor $[\ln(1+\beta)-\beta/(1+\beta)]$ in Eq. (4.8) is greater than unity for all $\epsilon\gtrsim\epsilon_s$, which are the energies of interest. Thus, for sufficiently strong magnetic fields the electron relaxation time may actually be increased by the presence of the magnetic field. We will show in the next section that this effect can give rise to a negative magnetoresistance under some circumstances.

In the appendix we give a simple theory of the screening lengths, $r_s{}^H$, $r_s{}^0$, in the presence and absence of the magnetic field, respectively. We find that in the case of classical statistics the magnetic field does not affect the screening length, whereas in the degenerate case it shortens it, according to the formula

$$(r_s{}^H/r_s{}^0)^2=N_0(\epsilon_F{}^0)/N(\epsilon_F{}^H)=2(\epsilon_F{}^0\epsilon_F{}^H)^{\frac{1}{2}}/\hbar\omega_0,$$

where $\epsilon_F{}^H$, $\epsilon_F{}^0$ are the Fermi energies with and without the magnetic field on, respectively.

V. LONGITUDINAL MAGNETORESISTANCE

We will now calculate the current induced by an electric field E in the z direction. We set up a Boltzmann equation for the distribution function $f(k_y,k_z)$ referring to the $N=0$ eigenstates of the electron in the magnetic field, i.e., $\psi(0k_yk_z;\mathbf{r})$. Since the magnetic field does not

affect the motion of the electron in the z direction, the electric field in the same direction simply accelerates the electron uniformly and thus

$$(\partial f/\partial t)_{\text{drift}}=(e/\hbar)E(\partial f/\partial k_z).$$

The steady state condition for the distribution function is then

$$(-e/\hbar)E(\partial f/\partial k_z)=(\partial f/\partial t)_{\text{coll}}.$$

For elastic collisions the scattering rate $(\partial f/\partial t)_{\text{coll}}$ is equal to $-(f-f_0)/\tau(\epsilon)$, where $f_0(\epsilon)$ is the distribution function for thermal equilibrium in the absence of the electric field and τ is the momentum relaxation time $-\dot{k}_z/k_z$ [see Eq. (3.2)]. We, therefore, have the following steady state equation:

$$\frac{e}{\hbar}E\frac{\partial f}{\partial k_z}=\frac{f-f_0(\epsilon_z)}{\tau_H(\epsilon_z)}. \tag{5.1}$$

To the first order in the field E, this integrates to

$$f(k_y,k_z)=f_0(\epsilon_z)+\frac{eE\hbar k_z}{m}\tau_H(\epsilon_z)\frac{df_0}{d\epsilon_z}. \tag{5.2}$$

The density of states with a given oscillator quantum number ($N=0$) and k_z in the range k_z, k_z+dk_z is

$$N(k_z)dk_z=\frac{2}{V}\frac{L_y}{2\pi}\frac{L_z}{2\pi}dk_z\int_{-(L_x/2\lambda^2)}^{+(L_x/2\lambda^2)}dk_y=\frac{2}{(2\pi)^2}\frac{1}{\lambda^2}dk_z, \tag{5.3}$$

as can be seen from Eq. (2.4). Thus, the current density in the z-direction is, according to Eqs. (2.7) (5.3), and (5.2),

$$J=(-e\hbar/m)\int k_z f(k_z)N(k_z)dk_z,$$

and, therefore,

$$\frac{J}{E}=\sigma_H=-\frac{2e^2}{m}\frac{1}{(2\pi)^2}\left(\frac{2m}{\hbar^2}\right)^{\frac{3}{2}}\hbar\omega_0\int_0^{\hbar\omega_0}\epsilon_z^{\frac{1}{2}}\tau_H(\epsilon_z)\frac{df_0}{d\epsilon_z}d\epsilon_z, \tag{5.4}$$

where σ_H is the zz-element of the conductivity tensor. Since the expectation values of the x and y components of velocity for our states vanish, the xz- and yz-elements of the conductivity tensor also vanish. Under such conditions it is easy to see that σ_H gives immediately the longitudinal magnetoresistance as measured in a long wire with the magnetic and electric fields along the wire. For, since $\sigma_{xz}=\sigma_{yz}=0$, we have $\rho_{zz}=1/\sigma_{zz}=1/\sigma_H$ and thus $\Delta\rho/\rho_0=(\sigma_0/\sigma_H)-1$.

By use of Eq. (5.3), the density of electrons is found to be

$$n_H=\frac{1}{(2\pi)^2}\left(\frac{2m}{\hbar^2}\right)^{\frac{3}{2}}\hbar\omega_0\int_0^{\hbar\omega_0}\epsilon_z^{-\frac{1}{2}}f_0(\epsilon_z)d\epsilon_z. \tag{5.5}$$

Similarly, in the absence of the magnetic field the distribution function, to the first order in E, is identical to the right-hand member of Eq. (5.2), except that $\tau_0(\epsilon)$ replaces $\tau_H(\epsilon_z)$ and ϵ now is the kinetic energy of the 3-dimensional motion of the electron. The conductivity and density of the electron gas are

$$\sigma_0=-\frac{2e^2}{m}\frac{2}{(2\pi)^2}\left(\frac{2m}{\hbar^2}\right)^{\frac{3}{2}}\int_0^\infty\epsilon^{\frac{3}{2}}\tau_0(\epsilon)\frac{df_0}{d\epsilon}d\epsilon, \tag{5.6}$$

$$n_0=\frac{2}{(2\pi)^2}\left(\frac{2m}{\hbar^2}\right)^{\frac{3}{2}}\int_0^\infty\epsilon^{\frac{1}{2}}f_0(\epsilon)d\epsilon. \tag{5.7}$$

We explicitly allowed in the above formulas for the possibility of change of carrier density with the introduction of the magnetic field. Although we shall not present here a detailed theory of this effect, we like to point out that the deepending of the impurity energy levels and the change of the density of states, both due to the magnetic field, can result in a substantial decrease of carrier concentration.

In general, of course, $1/\tau_H=(1/\tau_H{}^L)+(1/\tau_H{}^I)$ and similarly for the field-free case. Thus, the last four equations along with Eqs. (3.9), (3.11), (4.4), and (4.8) give us the conductivities of an electron gas in very strong and zero magnetic fields, in so far as ionized impurity and acoustical lattice scattering are the dominant relaxation mechanisms.

Below we shall discuss these results in the limiting cases of degenerate and classical statistics.

A. Degenerate Case

The degenerate case is that for which $\epsilon_F\gg kT$. If $\epsilon_F{}^0$ is the Fermi energy in the absence in the magnetic field, Eqs. (5.6) and (5.7) give

$$\sigma_0=(e^2/m)n_0\tau_0(\epsilon_F{}^0) \tag{5.8}$$

with

$$\epsilon_F{}^0=(3\pi^2)^{\frac{2}{3}}(\hbar^2/2m)n_0^{\frac{2}{3}}. \tag{5.9}$$

Similarly, if $\epsilon_F{}^H$ denotes the Fermi energy in the presence of the magnetic field, Eqs. (5.4) and (5.5) give

$$\sigma_H=(e^2/m)n_H\tau_H(\epsilon_F{}^H) \tag{5.10}$$

with

$$\epsilon_F{}^H=4\pi^4\left(\frac{\hbar^2}{2m}\right)^3\left(\frac{n_H}{\hbar\omega_0}\right)^2=\frac{4}{9}\left(\frac{n_H}{n_0}\right)^2\left(\frac{\epsilon_F{}^0}{\hbar\omega_0}\right)^2\epsilon_F{}^0. \tag{5.11}$$

In order for these expressions to be applicable, certain conditions have to be met. First, we must recall that all conduction electrons must be in the ground oscillator state; this is so if $\hbar\omega_0>\epsilon_F{}^H$. Also, $\epsilon_F{}^H\gg kT$ if the electron gas is to remain degenerate. Thus Eq. (5.10) is applicable only if

$$\hbar\omega_0>\frac{4}{9}\left(\frac{n_H}{n_0}\right)^2\left(\frac{\epsilon_F{}^0}{\hbar\omega_0}\right)^2\epsilon_F{}^0\gg kT.$$

If, therefore, a degenerate semiconductor ($\epsilon_F{}^0\gg kT$) is put into a magnetic field such that $\hbar\omega_0$ is of the order

of magnitude of $\epsilon_F{}^0$, most of the electrons will occupy the ground oscillator states and will be degenerately distributed. For $n_0 \sim 10^{18}$ cm^{-3} this requires a magnetic field $H \sim 3\times 10^5$ gauss, a value independent of the carrier mass. For much stronger magnetic fields the distribution is no longer degenerate and for much weaker fields the carriers are spread over the excited oscillator states.

When the condition for degeneracy is satisfied, we have

$$\frac{\sigma_H}{\sigma_0}=\frac{n_H}{n_0}\frac{\tau_H(\epsilon_F{}^H)}{\tau_0(\epsilon_F{}^0)}. \tag{5.12}$$

In the temperature range where acoustical scattering is predominant, Eqs. (3.9), (3.11), (5.11), and (5.12) give

$$\left(\frac{\sigma_H}{\sigma_0}\right)_L=\frac{4}{3}\left(\frac{n_H}{n_0}\right)^2\left(\frac{\epsilon_F{}^0}{\hbar\omega_0}\right)^2. \tag{5.13}$$

Equation (5.13) states that at sufficiently high fields the resistivity should be proportional to H^2. The H^2 dependence of ρ_H/ρ_0 is in contrast to the dependence expected from the classical theory, which predicts a value of ρ_H/ρ_0 independent of field. The dependence on H comes about as follows: $1/\tau_H{}^L$ is proportional to H for an electron with a given velocity; further, $1/\tau_H{}^L$ is inversely proportional to the velocity of the carriers and at high magnetic field the mean velocity decreases linearly with H on account of the increase of the density of oscillator ground states with H.

In the range of ionized-impurity scattering Eqs. (5.12), (4.4), and (4.8) give

$$\left(\frac{\sigma_H}{\sigma_0}\right)_I=\left(\frac{2}{3}\right)^3\left(\frac{n_H}{n_0}\right)^3\left(\frac{\epsilon_F{}^0}{\hbar\omega_0}\right)^3\frac{1+\beta_H}{\beta_H}\times\frac{\ln(1+\beta_0)-\beta_0/(1+\beta_0)}{I(\gamma_H)}, \tag{5.14}$$

where

$$\beta_H=4(\epsilon_F{}^H/\epsilon_s{}^H),\quad \gamma_H=(\epsilon_s{}^H/\hbar\omega_0)(1+\beta_H),$$
$$\beta_0=4\epsilon_F{}^0/\epsilon_s{}^0.$$

In the appendix we derive expressions for the energies $\epsilon_s{}^0$, $\epsilon_s{}^H$ associated with the screening, Eqs. (A.12) and (A.13).

For

$$\beta_0=(3\pi^5)^{\frac{1}{3}}a_0n_0{}^{\frac{1}{3}}\ll 1$$

($a_0=\kappa\hbar^2/e^2m$=Bohr's radius) expression (5.4) takes a simple form. For, then,

$$\beta_H=(2^4/3^3)(n_H/n_0)^3(\epsilon_F{}^0/\hbar\omega_0)^4\beta_0\ll 1$$

and

$$\gamma_H\cong(\epsilon_s{}^H/\hbar\omega_0)=(3/4)(n_0/n_H)(\hbar\omega_0/\epsilon_F{}^0).$$

In this range of γ_H, $I(\gamma_H)=1/(1+\gamma_H)$ and also

$$[\ln(1+\beta_0)-\beta_0/(1+\beta_0)]\cong\tfrac{1}{2}\beta_0{}^2.$$

We thus find that for $\beta_0\ll 1$

$$\left(\frac{\sigma_H}{\sigma_0}\right)_I=\frac{\beta_0}{4}\left(\frac{\hbar\omega_0}{\epsilon_F{}^0}\right)\left[1+\frac{3}{4}\left(\frac{n_0}{n_H}\right)\left(\frac{\hbar\omega_0}{\epsilon_F{}^0}\right)\right]. \tag{5.15}$$

B. Nondegenerate Case

If $kT\gg\epsilon_F$, nondegenerate statistics can be used. In this case the electron distribution takes the form

$$f_0(\epsilon)=\exp[(\epsilon_F{}^0-\epsilon)/kT].$$

Equations (5.4), (5.5), (5.6), and (5.7) then yield

$$\sigma_0=\frac{4e^2}{3\pi^{\frac{1}{2}}m}\left(\frac{n_0}{(kT)^{5/2}}\right)\int_0^\infty \epsilon^{\frac{3}{2}}\tau_0(\epsilon)e^{-\epsilon/kT}d\epsilon \tag{5.16}$$

and

$$\sigma_H=\frac{2e^2}{\pi^{\frac{1}{2}}m}\left(\frac{n_H}{(kT)^{\frac{1}{2}}}\right)\int_0^\infty \epsilon_z{}^{\frac{1}{2}}\tau_H(\epsilon_z)e^{-\epsilon_z/kT}d\epsilon_z. \tag{5.17}$$

The conditions for applicability of Eq. (5.17) will be always satisfied in the strong-field limit when

$$\hbar\omega_0\gg kT.$$

Numerically this condition requires a magnetic field $H\gg(kT/2\mu_B)\cong 10^4\alpha T$ gauss, where α is the ratio of effective to true electron mass.

In the range of predominantly lattice scattering we find, from Eqs. (3.9), (3.11), (5.15), and (5.16),

$$\left(\frac{\sigma_H}{\sigma_0}\right)_L=3\frac{n_H}{n_0}\left(\frac{kT}{\hbar\omega_0}\right). \tag{5.18}$$

Thus for a nondegenerate semiconductor in the quantum limit the longitudinal magnetoresistance in the lattice-scattering range, will exhibit a linear dependence on the magnetic field (assuming a negligible dependence of n_H on H), in contradistinction to the classical Boltzmann theory which predicts no magnetoresistance at all. It is worth noting that Eq. (5.18) would afford a determination of the effective mass of the carriers if (n_0/n_H) could be determined independently.

Assuming no compensation of impurities, we find from Eqs. (5.16), (5.17), (4.4), and (4.8) that when ionized impurity scattering is predominant,

$$\left(\frac{\sigma_H}{\sigma_0}\right)_I=\left[\ln(1+b_0)-\frac{b_0}{1+b_0}\right]\times\left[\frac{1}{2}+\frac{3}{4}\left(\frac{1}{b}\right)+3\frac{kT}{\hbar\omega_0}\left(2+\frac{4}{b}+\frac{3}{b^2}\right)\right]. \tag{5.19}$$

In obtaining this result, we have carried out the integration (5.16) assuming the logarithmic factor constant and equal to its value at the maximum of the rest of the integrand. Taking for $r_s{}^0$ the usual Debye screening

length, Eq. (A.15), we see that

$$b_0=12\frac{kT}{\epsilon_s{}^0}=\frac{6}{\pi}\left(\frac{m(kT)^2}{n_0\hbar^2e^2}\right). \tag{5.20}$$

In carrying out the integration (5.17), we have approximated $I(\gamma)$, appearing in $\tau_H{}^I(\epsilon_z)$, by $1/(1+\gamma)$, according to Eq. (4.7). From Eq. (A.14) for $r_s{}^H$, we see that in Eq. (5.19)

$$b=b_0(n_0/n_H). \tag{5.12}$$

An interesting feature of formula (5.19) is that for values of $b_0\gtrsim 1$, σ_H/σ_0 will usually exceed unity. Thus Eq. (5.19) indicates the possibility of a negative magnetoresistance in a simple electron gas.

Equation (5.19) is based on the usual Born approximation for the scattering, which is not always applicable. However, the possibility of negative magnetoresistance is a feature of this theory that is independent of the applicability of the Born approximation. The origin of the negative magnetoresistance is in the effect of the magnetic field to inhibit the small-angle scattering which in the field-free case is primarily responsible for momentum loss. Thus in the strong field the resistivity arises solely from the direct backward scattering, which is relatively weak.

VI. DISCUSSION

We will begin this section with a critique of our results and those of Titeica[2] and Davydov and Pomeranchuk,[3] who have considered certain facets of the strong-field problem. We will conclude with a discussion of the feasibility of a direct experimental observation of the effects.

The theory of Titeica is fairly extensive and is capable of comprehending a number of different cases. However, it contains implicitly one limitation which prevents its application to a number of cases of experimental interest. In all the treatment it is tacit that the Fermi energy is large, of the order of electron volts, as in a good metal. Perhaps because of this assumption, about the Fermi energy, the only scattering mechanism considered is acoustical lattice scattering. Thus, the applicability of the theory appears to be limited to good metals, or to semimetals and semiconductors at elevated temperatures. A feature of the theory which is unsatisfactory from the formal point of view is the failure to separate the scattering theory from the transport theory. Thus the calculation of the scattering rate for a carrier with a given set of quantum numbers is not separated from the calculation of the current carried by an ensemble.

The work of Titeica was designed to be useful in discussing magnetoresistance experiments on good metals at fields of several hundred kilooersted. For such experiments the magnetic energy quantum $\hbar\omega_0$ would normally remain well below 0.1 ev, while the electron energies would range up to values more than an order of magnitude greater. Thus the extreme quantum limit would be unattainable, and most electrons will occupy states of fairly high oscillator quantum number. Thus the part of the theory which admits of experimental comparison is the treatment of high magnetic fields, which are, however, inadequate to reach the quantum limit.

The theory of Davydov and Pomeranchuk is a theory of quantum effects on relaxation in a semimetal, and so assumes the Fermi energy to be small. These authors are interested in interpreting experiments on strong-field magnetoconductivity of bismuth, a substance in which the effective mass is very small, and the experimental possibility of reaching the quantum limit exists. They are concerned chiefly with the interpretation of certain oscillations in the resistivity as a function of magnetic field together with the notable nonsaturation behavior at the highest fields. Their qualitative interpretation of the former is doubtless correct, but the treatment of the latter is open to some objection.

In this theory it is assumed that the mobility is determined chiefly by the scattering from ionized impurities. The scattering potential of such an ionized impurity is effectively taken to be a delta function in position, and the scattering matrix elements calculated on this basis.

Now it is a fact that the scattering matrix elements calculated from a delta function potential are typical of acoustical rather than Coulomb scattering. Thus the theoretical model of Davydov and Pomeranchuk would yield $\tau\propto\epsilon^{-\frac{1}{2}}$ rather than $\tau\propto\epsilon^{\frac{3}{2}}$ as on the customary theories of ionized impurity scattering or $\tau\propto\epsilon^0$ on the theory of neutral impurity scattering. Since the behavior of the resistivity in the quantum limit is very sensitive to the scattering mechanism, the delta function approximation would appear unsatisfactory.

The present work is limited in scope to materials of very low electron concentration and low temperatures. We choose to discuss a set of cases which are similar to those in n-type InSb which seems particularly well suited for the study of the quantum limit. Our aim in the calculation was not so much to predict the outcome of experiments done in the quantum limit as to determine the degree to which the outcome is sensitive to scattering mechanism.

We find that the field dependence of the relaxation time in the quantum limit is very sensitive to the mechanism responsible for scattering. Thus, for lattice scattering the magnetoresistance is always positive, but for impurity scattering a negative magnetoresistance is to be expected under some circumstances.

In order to best observe the quantum effects experimentally, the material of choice is a semiconductor or a semimetal in which the electron mass is very small. A good example is n-type InSb, and we will consider it for illustrative purposes.

According to Kittel *et al.*, the effective mass in InSb is about 1/70 of an electron mass. Thus for a magnetic field of 5×10^5 gauss the magnetic quantum would have a value, in temperature units, of about 4000°K. Fields of such magnitude are currently produced in the laboratory and used for quasistatic measurements of the sort discussed in this paper. Clearly an energy of 4000°K is more than adequate to permit studies under the condition $\hbar\omega_0 \gg kT$ even at room temperature.

The concentrations of carriers needed to realize the conditions assumed in our calculation are easily achieved in practice. The relation between degeneracy temperature and concentration for InSb is

$$T_D \sim 2\times10^{-9} n^{\frac{2}{3}} \text{ °K}.$$

This formula gives for $n\sim10^{14}$ a degeneracy temperature of 4°K; for $n\sim10^{15}$, $T_D\sim20$°K; for $n\sim10^{16}$, $T_D\sim90$°K; for $n\sim10^{17}$, $T_D\sim400$°K. These concentrations and temperatures at once span the range of compositions over which it is feasible to prepare single-crystal specimens and that over which it is feasible to make precise electrical measurements.

We will not make any interpretation of experimental results in this paper, because of various questions having to do with the applicability of our models to those experiments which are available. However, we will point out that Sladek and Keyes at Westinghouse and Frederickse[4] at the National Bureau of Standards have made measurements of the electrical conductivity of InSb in strong magnetic fields and have found effects of the qualitative nature and of the same order of magnitude as those expected on our theory.†

APPENDIX

We present here a simple theory of the screening lengths appropriate for the ionized impurity scattering under the conditions considered in this paper.

Let $v(\mathbf{r})$ be the self-consistent energy of an electron at a point $\mathbf{r}$ from a point charge $(\pm e)$ placed in our unperturbed system, i.e., an electron gas of density n_H electrons per unit volume in a magnetic field H strong enough to force all electrons in the ground oscillator states. The electron gas is held together by the lattice positive charge density $+en_H$. If $n(\mathbf{r})$ is the electron density at $\mathbf{r}$ when equilibrium has been reached after the introduction of the impurity the self-consistent potential energy $v(\mathbf{r})$ must satisfy Poisson's equation

$$\nabla^2 v(\mathbf{r}) = -\frac{4\pi e^2 n_H}{\kappa}\left[\frac{n(\mathbf{r})}{n_H}-1\right], \tag{A.1}$$

where κ is the dielectric constant of the lattice.

We can determine the particle density $n(\mathbf{r})$ in terms of $v(\mathbf{r})$ under the simplifying assumption that $v(\mathbf{r})$ is such a slowly varying function of position that we can treat its effects on the unperturbed system classically, i.e., we may assume that at every point the system behaves as if a constant potential energy, equal to the local value of $v(\mathbf{r})$, were added to the energy of the system. We can then take, for the energies of the perturbed system,

$$\epsilon'(\mathbf{r},k_z) = v(\mathbf{r}) + \epsilon_z.$$

With this assumption,

$$n(\mathbf{r}) = 2\sum_{k_y k_z} |\psi(0k_y k_z;\mathbf{r})|^2 f(\epsilon'),$$

where $f(\epsilon')$ is the Fermi probability function. Using Eqs. (2.3) and (2.5), we see that

$$\sum_{k_y} |\psi(0k_y k_z;\mathbf{r})|^2 = \frac{1}{L_z}\left(\frac{1}{2\pi}\right)\left(\frac{1}{\lambda^2}\right),$$

and with the help of Eq. (5.3) we can write

$$n(\mathbf{r}) = \int_0^\infty f(v+\epsilon_z) N(\epsilon_z)\, d\epsilon_z, \tag{A.2}$$

where

$$N(\epsilon_z) = \frac{1}{(2\pi)^2}\left(\frac{2m}{\hbar^2}\right)^{\frac{3}{2}} \hbar\omega_0 \epsilon_z^{-\frac{1}{2}} \tag{A.3}$$

is the density of states with energy $\epsilon' = v+\epsilon_z$ per unit energy interval. The particle density in the absence of the impurity is obtained from Eq. (A.2) for $v=0$, i.e.,

$$n_H = \int_0^\infty f(\epsilon_z) N(\epsilon_z)\, d\epsilon_z, \tag{A.4}$$

and this determines the constant Fermi level.

For the case $H=0$, we similarly have

$$\nabla^2 v(\mathbf{r}) = -\frac{4\pi e^2 n_0}{\kappa}\left[\frac{n_0(\mathbf{r})}{n_0}-1\right], \tag{A.5}$$

where now

$$\frac{n_0(\mathbf{r})}{n_0} = \int_0^\infty f(v+\epsilon) N_0(\epsilon)\, d\epsilon \Big/ \int_0^\infty f(\epsilon) N_0(\epsilon)\, d\epsilon \tag{A.6}$$

with

$$N_0(\epsilon) = [2/(2\pi)^2](2m/\hbar^2)^{\frac{3}{2}}\epsilon^{\frac{1}{2}}. \tag{A.7}$$

Degenerate statistics.—In this case Eqs. (A.2), (A.4), and (A.6) give

$$\frac{n(\mathbf{r})}{n_H} = \frac{\int_0^{(\epsilon_F{}^H - v)} \epsilon_z^{-\frac{1}{2}} d\epsilon_z}{\int_0^{\epsilon_F{}^H} \epsilon_z^{-\frac{1}{2}} d\epsilon_z} = \left[1-\frac{v(\mathbf{r})}{\epsilon_F{}^H}\right]^{\frac{1}{2}} \tag{A.8}$$

[4] R. J. Sladek and R. W. Keyes (private communication) and H. P. R. Frederickse (private communication).

† *Note added in proof.*—Results similar to some of ours have been recently reported by Dr. J. Appel of OSRAM, Augsburg, and Professor R. Kubo of the University of Tokyo (private communication).

and

$$\frac{n_0(\mathbf{r})}{n_0}=\left[1-\frac{v(\mathbf{r})}{\epsilon_F{}^0}\right]^{\frac{3}{2}}. \tag{A.9}$$

The resulting Poisson's equations can be solved simply under the additional assumption that $|v(\mathbf{r})/\epsilon_F|\ll 1$. For then Eqs. (A.1) and (A.5) become of the form

$$\nabla^2 v(\mathbf{r})=a^2 v(\mathbf{r}). \tag{A.10}$$

The solution of this equation with the appropriate boundary conditions

$$v(\mathbf{r})\underset{r\to 0}{\longrightarrow}\pm\frac{e^2}{\kappa}\left(\frac{1}{r}\right),\quad v(\mathbf{r})\underset{r\to\infty}{\longrightarrow}0,$$

is

$$v(\mathbf{r})=\pm\frac{e^2}{\kappa}\left(\frac{e^{-ar}}{r}\right), \tag{A.11}$$

which is the screened Coulomb potential used in our calculations with $a=1/r_s$.

It is easily seen that

$$\frac{1}{(r_s{}^H)^2}=\frac{4\pi e^2}{\kappa}\left(\frac{n_H}{2\epsilon_F{}^H}\right)=\frac{e^2}{\pi\kappa}\left(\frac{2m}{\hbar^2}\right)^{\frac{3}{2}}\left(\frac{\hbar\omega_0}{(\epsilon_F{}^H)^{\frac{1}{2}}}\right) \tag{A.12}$$

and

$$\frac{1}{(r_s{}^0)^2}=\frac{4\pi e^2}{\kappa}\left(\frac{n_0}{(2\epsilon_F{}^0/3)}\right)=\frac{2e^2}{\pi\kappa}\left(\frac{2m}{\hbar^2}\right)^{\frac{3}{2}}(\epsilon_F{}^0)^{\frac{1}{2}}. \tag{A.13}$$

Classical statistics.—In this case it is clear that since

$$f(v+\epsilon_z)\sim e^{-v(\mathbf{r})/kT}e^{-\epsilon_z/kT}$$

we get

$$\frac{n(\mathbf{r})}{n_H}=\frac{n_0(\mathbf{r})}{n_0}=e^{-v(\mathbf{r})/kT}\cong 1-\frac{v(\mathbf{r})}{kT}$$

(for $|v(\mathbf{r})/kT|\ll 1$), and thus Poisson's equation for both cases is again of the form (A.10). Hence, the self-consistent potential energy is again of the form (A.11), with

$$\frac{1}{(r_s{}^H)^2}=\frac{4\pi e^2}{\kappa}\left(\frac{n_H}{kT}\right) \tag{A.14}$$

and

$$\frac{1}{(r_s{}^0)^2}=\frac{4\pi e^2}{\kappa}\left(\frac{n_0}{kT}\right). \tag{A.15}$$

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Variation of the Amplitude of Thermal Vibration on the Fusion Curve

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A differential relation given previously, which is equivalent to the Debye-Waller identification of the Debye and Lindemann frequencies at fusion, is generalized to take into account variation along the fusion curve of the critical ratio of the root-mean-square amplitude of thermal vibration to the nearest-neighbor distance of the atoms in the solid at fusion. Thus extended, the theory yields an expression for the Grüneisen parameter of a solid at fusion in terms of fusion parameters and the rate of change of the critical ratio with respect to volume, which is valid for elements whose fusion curves have either normal or abnormal slopes. Values of derivatives of the critical ratio with respect to volume, temperature, and pressure at fusion are obtained for 16 elements. The results yield evaluations of the change in the critical ratio along the experimentally determined fusion curves for three alkali metals, and permit estimates in other cases. It is concluded that the assumption of a fixed Lindemann constant along the fusion curve of a particular element represents an excellent approximation, in general, for elements with normal fusion curves (for the case of classical excitation of the lattice vibrations). The same conclusion is obtained, within certain approximations, from the order-disorder theory of Lennard-Jones and Devonshire for the melting process, and the theory of Fisher for stability of the liquid phase.

I. INTRODUCTION

IT has been pointed out by the author[1] and by Cartz[2] that the Lindemann law of melting can be derived under certain assumptions from the Debye-Waller theory of the thermal dependence of the intensity of Bragg reflection of x-rays from a solid. In a recent paper, the author obtained relatively accurate values of Lindemann constants, and thus of amplitudes of thermal vibration for the solid at melting, from the Debye-Waller theory for ten elements.[3] The results show that the Lindemann constant, and hence the critical ratio of the root-mean-square amplitude of thermal vibration to the nearest-neighbor distance of the

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