High-magnetic-field thermopower in a layered superlattice

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The electron diffusion contribution to the thermoelectric power is calculated for a layered superlattice in a high magnetic field. The shape of the quantum oscillations is shown to depend significantly on the ratio of the temperature to the interlayer bandwidth (W) divided by Boltzmann's constant (k_B). When the highest occupied Landau level is partially filled, the thermopower is linear in temperature at low temperatures and saturates to a constant value for temperatures approximately comparable to or larger than Wk_B^{-1}. When the highest occupied Landau level is nearly filled, the thermopower occurs via activation to the adjacent higher level. The effect of electron localization is discussed. This study provides useful information about some of the important properties of layered superlattices, such as the carrier densities, the Fermi temperatures, the electronic structures in the superlattice direction, and the effect of carrier localization.

I. INTRODUCTION

The thermoelectric phenomenon gives valuable information about electron-transport processes in metals and semiconductors. In this paper we study the temperature-dependent and the magnetic-field-dependent behaviors of the thermoelectric effect in quasi-two-dimensional systems such as layered superlattices and heterostructure inversion layers, which are the subject of increasing current activities.[1] We deal mainly with superlattices while an inversion layer is treated merely as a special two-dimensional case where the interlayer overlap vanishes. In the latter case the detailed form of the potential well in the direction perpendicular to the layer does not affect the final result. These systems are characterized by a nearly two-dimensional metallic conduction with very low Fermi temperatures less than a few hundred degrees kelvin and with low densities of carriers compared to ordinary metals. As a result a large electron-diffusion thermopower is expected in comparison to ordinary metals, although it is smaller than that in a nondegenerate semiconductor. Apart from an academic interest it is hoped that this study will provide useful means of looking into some of the important properties of layered superlattices such as the carrier densities, Fermi temperatures, electronic structures in the superlattice direction, and the effect of carrier localization.

This study is applicable to a wide variety of quasi-two-dimensional systems. A good example is the strained layer superlattice $In_xGa_{1-x}As/GaAs$ where large-amplitude quantum oscillations in the magnetotransport were observed recently by Shirber *et al.*[2] This system consists of alternating sheets of conducting and insulating layers of widths on the order of 250 Å or less, each forming quantum wells and barriers stacked in the superlattice direction. Electrons are then introduced by Si doping with layer densities $n_s=(1-8)\times10^{11}$ cm^{-2} corresponding to the Fermi temperatures in the range $T_F=30-300$ K. For an effective mass $m/m_0=0.06$ and a quantum-well width of 125 Å, for example, the energy separation between the ground and first excited subbands is about 1400 K. Therefore, only the ground subband is assumed to be occupied at low temperatures in the following analysis. The bandwidth (W) in the superlattice direction is small, roughly on the order of $W=(50\text{ K})k_B$ or smaller. Here, k_B is Boltzmann's constant. Later applications are made with the above physical parameters in mind.

The magnetic field ($\vec{H}$) is assumed to be in the superlattice direction (to be designated as the z axis). Because of the small effective mass, the cyclotron angular frequency (ω) is quite large for a moderate field. For example, for $H=40$ kG the Landau-level separation equals $\hbar\omega=\hbar eH/mc=(88.8\text{ K})k_B$ where e and c are the electronic charge and the speed of light. The field is assumed to be sufficiently large to be in the quantum limit, namely,

$$\hbar\omega \gg k_BT \tag{1.1}$$

and

$$\omega\tau \gg 1 . \tag{1.2}$$

Here, τ is the transport relaxation time for the electrons. These conditions are readily satisfied in the superlattice cited above.[2]

The energy of an electron is given by

$$\epsilon(\vec{H})=(l+\tfrac{1}{2})\hbar\omega+\epsilon_{k_z} , \tag{1.3}$$

where l is an integer. An application will be made to a tight-binding model with the kinetic energy in the z direction given by

$$\epsilon_{k_z}=W[1-\cos(k_za)]/2 . \tag{1.4}$$

Here k_z and a are the momentum and electronic period in the superlattice direction, respectively. A general band structure in the z direction can be easily treated numerically. Here we do not necessarily assume a coherent motion in the z direction. The degeneracy of the Landau levels (including spin) equals

$$g=eHL^2/\pi\hbar c , \tag{1.5}$$

where L^2 is the area of the conducting x-y plane.

The temperature gradient is in the x direction in the conducting plane. The temperature gradient produces an electric field mainly in the same direction if the electric current is not allowed to flow. We study the temperature dependence and the field dependence (i.e., quantum oscillations) of the electron-diffusion contribution to the thermoelectric power. The effect of a finite interlayer bandwidth is examined.

The organization of this paper is as follows. In Sec. II a basic formalism of the thermopower is introduced. This result is used in Sec. III to investigate the electron-diffusion thermopower. A brief conclusion is given in Sec. IV.

II. BASIC FORMALISM

The charge and heat currents $\vec{J}$ and $\vec{U}$ are written in a linear-response regime as a linear combination of the electric field $\vec{E}$ and the temperature gradient[3]

$$\vec{J}=\overleftrightarrow{\sigma}(\vec{H})\cdot\vec{E}+\overleftrightarrow{L}_{ET}(\vec{H})\cdot\vec{\nabla}T\ , \tag{2.1a}$$

$$\vec{U}=\overleftrightarrow{L}_{TE}(\vec{H})\cdot\vec{E}+\overleftrightarrow{L}_{TT}(\vec{H})\cdot\vec{\nabla}T\ , \tag{2.1b}$$

where the proportionality coefficients represent second-rank tensors. The Onsager relationship yields[3]

$$\overleftrightarrow{L}_{ET}(\vec{H})=-\overleftrightarrow{\tilde{L}}_{TE}(-\vec{H})/T \tag{2.2}$$

with the tilde meaning the transpose.

The tensors in (2.1) except for $\overleftrightarrow{L}_{TT}$ are mainly off diagonal, namely, the electronic heat and charge currents are in the transverse (i.e., y) direction due to deflection by a Lorentz force. If the electric current is not allowed to flow in the y direction (i.e., $J_y=0$), the off-diagonal terms in (2.1a) yield in view of the Onsager relation (2.2) a thermoelectric power

$$S(\vec{H})=E_x/\vec{\nabla}_x T=\frac{L_{TE}^{yx}(\vec{H})}{\sigma_{yx}(\vec{H})T}\ . \tag{2.3}$$

Here, use is made of the relationship

$$\tilde{L}_{TE}^{yx}(-\vec{H})=L_{TE}^{xy}(\vec{H})\ .$$

In (2.3) a small contribution arising from a finite-temperature gradient in the y direction present under the usual adiabatic boundary condition ($U_y=0$) is ignored.[4] The problem is then reduced to calculating the ratio of the transverse heat and charge currents per temperature for an electric field in the x direction in the absence of the temperature-gradient term in (2.1).

III. THERMOELECTRIC POWER

The contribution to the electrical conductivity and the heat current tensors $\overleftrightarrow{\sigma}(\vec{H})$ and $\overleftrightarrow{L}_{TE}(\vec{H})$ is conveniently expressed in terms of the energy-dependent conductivity tensor $\overleftrightarrow{\sigma}(\epsilon)$ [to be distinguished from $\overleftrightarrow{\sigma}(\vec{H})$] by

$$\overleftrightarrow{\sigma}(\vec{H})=\int[-f^{0'}(\epsilon)]\overleftrightarrow{\sigma}(\epsilon)d\epsilon\ , \tag{3.1a}$$

$$\overleftrightarrow{L}_{TE}(\vec{H})=(1/e)\int f^{0'}(\epsilon)(\epsilon-\mu)\overleftrightarrow{\sigma}(\epsilon)d\epsilon\ , \tag{3.1b}$$

where $f^{0'}$ and μ are the derivatives of the Fermi function and the chemical potential. In a strong field [cf. (1.2)] we need only the Hall conductivity tensor

$$\sigma_{yx}(\epsilon)=\frac{n(\epsilon)ec}{H\Omega}\ . \tag{3.2}$$

In (3.2) $n(\epsilon)$ is the number of the states within the energy shell ϵ for the sample of volume Ω,

$$n(\epsilon)=\int_0^{\epsilon}D(\epsilon')d\epsilon' \tag{3.3}$$

and $D(\epsilon)$ is the density of states.

Inserting (3.1)—(3.3) into (2.3) we find

$$S(\vec{H})=-(1/eTN)\int[-f^{0'}(\epsilon)](\epsilon-\mu)n(\epsilon)d\epsilon\ , \tag{3.4}$$

where N is the total number of electrons

$$N=\int f^0(\epsilon)D(\epsilon)d\epsilon\ . \tag{3.5}$$

In the above we have assumed that σ_{xx} is negligible compared with σ_{xy} for $\omega\tau\gg1$, which is not valid in the extreme disordered limit. The present semiclassical approach is valid for static disorder. Note that the quantity $n(\epsilon)$ in the integral of (3.4) is not the usual density of states which enters the field-free thermopower formula but an integration of the density of states [cf. (3.3)]. Nevertheless, the dominant contribution to the heat flow still comes from the states near the Fermi level as in the field-free situation owing to the "electron-hole" cancellation factor $\epsilon-\mu$. On the other hand, all states inside the Fermi surface contribute to the Hall current ($\propto N$) in the denominator of (3.4) in contrast to the field-free case where the concomitant charge current in the denominator reflects the contribution only from states near the Fermi level. For this reason the low-temperature magnetothermopower becomes very small when the Fermi level lies in the gap or in the region of localized states, whereas the field-free thermopower is very large, as in semiconductors in this situation.

In the presence of the Landau levels, the density of states is written as

$$D(\epsilon)=(gN_z/\pi)\int_0^{\pi}d(k_za)\sum_{l=0}^{\infty}\delta(\epsilon-\hbar\omega(l+\tfrac{1}{2})-\epsilon_{k_z})\ , \tag{3.6}$$

which yields for the tight-binding band in (1.4)

$$D(\epsilon)=(gN_z/\pi W^2)\sum_{l=0}^{\infty}[(W+\hbar\omega(l+\tfrac{1}{2})-\epsilon)\times(\epsilon-\hbar\omega(l+\tfrac{1}{2}))]^{-1/2}\ . \tag{3.7}$$

Here, N_z is the number of periods in the superlattice direction.

The chemical potential is obtained as a function of N in the following way.[5] Let l_F be the number of occupied Landau levels. The chemical potential then lies between $\hbar\omega(l_F-\frac{1}{2})$ and $\hbar\omega(l_F+\frac{1}{2})$. Assuming that the Landau levels do not overlap and that $\hbar\omega-W\gg k_BT$ for simplicity, we need to consider only the levels $l=l_F-1$ and l_F in (3.6) separately. Otherwise, the level $l=l_F-2$ should

be included. Inserting (3.6) into (3.5), we find

$$B=\frac{1}{\pi}\int_0^{\pi} d(k_z a)\sum_{\pm}\frac{1}{e^{z\pm}+1},\quad z_{\pm}=\beta\epsilon_{k_z}+x\pm y \quad (3.8)$$

where $\beta^{-1}=k_B T$ and B is the occupancy of the highest occupied level ($0\le B<1$) given in terms of the filling factor p by

$$B=p-[p],\quad p=N/gN_z \quad (3.9)$$

with $[p]$ meaning rounding off p to an integer value. The quantities x and y in (3.8) are defined by

$$x=\beta(\hbar\omega l_F-\mu),\quad y=\beta\hbar\omega/2\ . \quad (3.10)$$

In the limit $\beta W\ll 1$, (3.8) yields[5]

$$x=\ln\{[(1-B)\cosh y+(1+(1-B)^2\sinh^2 y)^{1/2}]/B\}\ . \quad (3.11)$$

At extreme low temperatures [i.e., $k_B TD(\mu)\ll 1$] the expression in (3.4) reduces in view of (3.3) to

$$S(\vec{H})=-\pi^2 k_B^2 TD(\mu)/3eN\ . \quad (3.12)$$

Here, the Fermi level is assumed to lie in the conducting region. Otherwise the thermopower is exponentially small as argued above. Another way of justifying this claim is to use Mott's formula

$$S(H)\propto\frac{\partial\ln\sigma_{yx}(\mu)}{\partial\mu}$$

[obtained from (2.3), (3.1), and (3.2)] which vanishes in the quantum Hall effect plateau regime. The thermopower is then proportional to the density of states at the Fermi level. For the tight-binding band in (1.4) the chemical potential is obtained from (3.8) and equals

$$y-x=\beta W\sin^2(\pi B/2)\ ,$$

yielding for (3.7) and (3.12),

$$D(\mu)/N=2[\pi pW\sin(\pi B)]^{-1}\ . \quad (3.13)$$

The thermopower is then given by

$$S(\vec{H})=\frac{S_0}{p\sin(\pi B)},\quad S_0=-2\pi k_B^2 T/3eW\ . \quad (3.14)$$

In Fig. 1 the thermopower is plotted in units of S_0 as a function of the filling factor p. The latter equals unity, for example, for $H=40$ kG and $n_s=2.0\times 10^{11}$ cm^{-2}. All states are assumed to be conducting in the x-y plane. If there is any mobility edge, the thermopower drops to zero in the localized region. If all states below the Fermi level are localized, as may occur in the extreme quantum limit ($p>1$), then both heat and Hall currents are via activation to the mobility edge. The thermopower is then large as in a semiconductor. In Fig. 1 the Landau levels are assumed not to overlap (i.e., $\hbar\omega>W$). For large values of p, namely, for small fields they will eventually overlap and the thermopower as well as the density of states [cf. (3.7)] will rise near each band edge as in Fig. 1 showing more structures.

In general the thermopower is given by (3.4) with

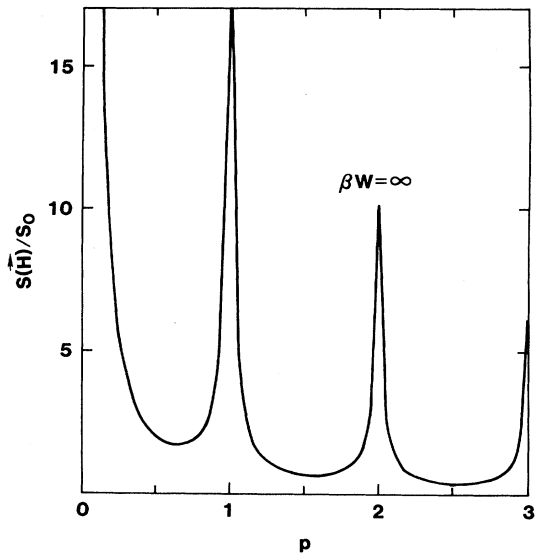

FIG. 1. Very-low-temperature thermopower in units of S_0 [cf. (3.14)] vs the filling factor p.

$$n(\epsilon)=(N/p\pi)\int_0^{\pi} d(k_z a)\sum_{l=0}^{\infty}\Theta(\epsilon-\epsilon_l) \quad (3.15a)$$

and

$$\epsilon_l=\hbar\omega(l+\tfrac{1}{2})+\epsilon_{k_z}\ , \quad (3.15b)$$

where $\Theta(x)$ is a unit step function. In the limit $\beta W\ll 1$ the expression in (3.4) reduces to the two-dimensional result.[6] The quantity $n(\epsilon)$ in (3.15) can be viewed as a sum of steplike densities of states which are independent of energy for $\epsilon>\epsilon_l$. If we assume $\beta(\hbar\omega-W)\gg 1$, then the integrand in (3.4) becomes approximately symmetric for $l<l_F-1$ and the net contribution is negligible. On the other hand, the contribution from $l>l_F$ is exponentially small. Therefore retaining only $l=l_F-1$ and l_F, we find

$$S(\vec{H})=-\frac{k_B}{ep\pi}\int_0^{\pi} d(k_z a)\sum_{j=+,-}\left[\frac{z_j}{e^{z_j}+1}+\ln(1+e^{-z_j})\right]. \quad (3.16)$$

The high-temperature ($\beta W\ll 1$) thermopower can be evaluated analytically. When the occupancy B is nearly unity, we find from (3.11) and (3.16) a very small thermopower

$$S(\vec{H})=-4k_B y e^{-y}/ep\ . \quad (3.17)$$

In this case, the Fermi level lies halfway between two Landau levels (i.e., $x=0$). For a filled band the entropy (i.e., heat per temperature) vanishes and heat can be carried only by activation to the next level.

When the highest occupied Landau level is partially filled [i.e., $1-B\gg\exp(-y)$], we find from (3.11) and (3.16)

$$S(\vec{H})=-\frac{k_B}{ep}\left[B\ln\frac{1-B}{B}-\ln(1-B)\right]. \quad (3.18)$$

The quantity in the large parentheses of (3.18) is sym-

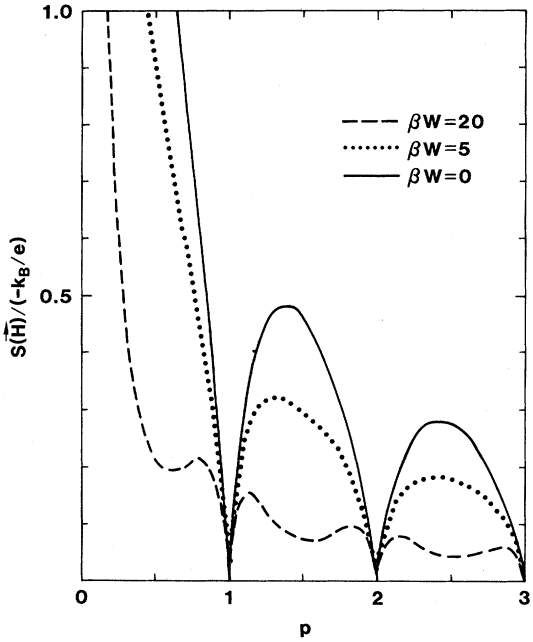

FIG. 2. Thermopower vs the filling factor p for $\beta W=0$ (solid curve), $\beta W=5$ (dotted curve), and $\beta W=20$ (dashed curve).

metric with respect to $B=\frac{1}{2}$ with a peak value of ln2 and vanishes as $B\ln B^{-1}$ at $B=0$. This behavior reflects the fact that the entropy and thus the heat flow becomes maximum (i.e., ln2 per state) at half-filling of the band and drops as the band is gradually emptied or filled.

In Fig. 2 the high-temperature thermopower is plotted in a solid curve as a function of the filling factor p. The filling factor p can be varied either by changing the magnetic field or by changing the electron density, yielding the same curve independent of the temperature except at near the exact filling. For the latter, however, the thermopower is negligibly small as was noted in (3.17).

For intermediate values of the interlayer bandwidth W Eqs. (3.8) and (3.16) are evaluated numerically. The results are displayed in Fig. 2 in a dashed curve for $\beta W=20$ and a dotted curve for $\beta W=5$. The curves clearly display a gradual change from a two-dimensional behavior ($\beta W=0$) to a three-dimensional behavior ($\beta W=\infty$) exhibited in Fig. 1. The shape of the quantum oscillations

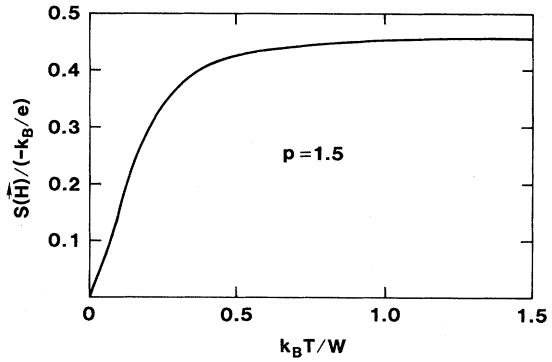

FIG. 3. Thermopower vs the reduced temperature for $p=1.5$.

depend significantly on the ratio of the temperature to Wk_B^{-1}.

Finally the thermopower is plotted as a function of the temperature in Fig. 3 for $p=1.5$. The latter corresponds, for example, to $H=40$ kG and $n_s=3.0\times10^{11}$ cm^{-2}. The thermopower is linear at low temperatures as in (3.12) and saturates to a constant value near $\beta W=1$. At integer values of p the thermopower occurs via activation [cf. (3.17)].

IV. CONCLUSION

The electron-diffusion contribution to the thermoelectric power was examined for a layered superlattice in a high-magnetic field. The shape of the quantum oscillations was shown to depend significantly on the ratio of k_BT to the interlayer bandwidth. When the highest occupied Landau level is partially filled, the thermopower is linear in temperature at low temperatures and saturates to a constant value for k_BT larger than the interlayer bandwidth. When the highest occupied level is nearly filled, the thermopower occurs via activation to the adjacent higher level. The effect of electron localization was discussed.

ACKNOWLEDGMENTS

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