Transport Coefficients Based on Magneto Translationally Invariant Wave Functions*

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(Received 5 November 1968; revised manuscript received 27 January 1970)

A general theory of quantum magnetotransport effects for conduction electrons, with emphasis on the consequences of Harper broadening, yields new expressions for a magnetic-field-dependent effective mass and finite-wavelength conductivity coefficients. An examination of the conductivity coefficient relevant to magneto acoustic Doppler-shifted cyclotron resonance experiments reveals the presence of peaks in the sound-wave attenuation coefficient beyond the absorption edge. The analysis includes the use of density-matrix techniques with a representation that is simultaneously an eigenfunction of the Bloch Hamiltonian (for an electron in a uniform magnetic field) and the magnetic translation operators. The eigenfunctions, eigenvalues, and conductivity coefficients are studied for an orthorhombic system and then specialized to the case when the crystalline potential has the form $V(x, y, z) = V(x, y) + V(z)$ (the magnetic field is along z). Contributions due to Harper broadening are isolated. Estimates of the magnetic-field dependence of the conductivity coefficients are presented.

I. INTRODUCTION

In 1955 Harper[1] pointed out a significant omission in the semiclassical treatment of conduction electrons in uniform magnetic fields. This was the periodic potential broadening of the quantized-oscillator levels. Since then the consequences of potential-broadened levels has been studied by Pippard[2] and others[3] who have examined the relation between this effect and magnetic-breakdown phenomena.[4] However, general treatments of quantum magnetotransport effects incorporating potential broadening in a natural way have not appeared. The main difficulty, perhaps, was in the selection of representations that adequately described the basic symmetry of the problem. For the case of zero magnetic field, Bloch functions provide a natural basis. For finite magnetic fields and zero periodic potential, Landau functions are appropriate. For finite magnetic fields and finite crystalline potential, the representation of Harper and more recently those of Zak[5] and Brown[6] describe in a natural way the invariance properties of the crystal.[7] The important feature of these latter representations is the notion of crystalline energy bands in the presence of uniform fields, these bands being a direct consequence of translational symmetry of the crystal in uniform magnetic fields.

In this paper a general treatment of quantum magnetotransport effects for electrons in crystalline solids is presented using a representation similar to those of Harper, Zak, and Brown. The consequences of the broadened levels for electrons subject to space- and time-dependent fields is examined. Examples from magnetoacoustics are used to illustrate principal new effects. Among the results, a particularly interesting one occurs for a shear wave propagating parallel to the magnetic field. Here we demonstrate the presence of peaks[8] in the sound-wave attenuation coefficient *beyond* the absorption edge[9] with amplitudes related to the width of the broadened levels.

To formulate the problem, density-matrix techniques are used. These techniques are patterned after the work of Tosima, Quinn, and Lampert.[10] While the results are superficially similar in form to the free-electron calculation of Tosima *et al.*, they are exact and sufficiently general to yield results due to the effects of broadened levels, as well as those due to ordinary magnetic-field-dependent phenomena. The basis functions for the purpose are simultaneous eigenfunctions of the Hamiltonian

$$\mathcal{H}_0 = (1/2m)(\vec{p} - e\vec{A}_0/c)^2 + V(\vec{r}) \quad , \tag{1.1}$$

and the magnetic translation operators (MTO)

$$\tau(\vec{R}_n) = \exp i[(\vec{p} + e\vec{A}_0/c)\cdot \vec{R}_n/\hbar] \tag{1.2}$$

for a particle in a uniform field $\vec{B}$ of charge e, mass m, and crystalline potential $V(\vec{r}) = V(\vec{r} + \vec{R}_n)$. Here $\vec{R}_n$ is a lattice vector and $\vec{A}_0 = \frac{1}{2}\vec{B} \times \vec{r}$. The eigenfunctions and eigenvalues of the Hamiltonian are denoted, respectively, by $\psi(\vec{r}; n\vec{\kappa}\sigma)$ and $\epsilon(n, \vec{\kappa})$ and interpretation is in terms of a band picture. n denotes the band index and $\vec{\kappa}$ the wave vector. The properties of the eigenfunctions and eigenvalues of the above equations as well as those of relevant matrix elements are discussed in Sec. II.[11]

In Sec. III, we construct single-particle density-matrix elements for conduction electrons in uniform magnetic, and space- and time-dependent electric fields. In Sec. IV magnetic-field-dependent, frequency-dependent, and wavelength-dependent conductivity coefficients are obtained from Fourier-transformed ensemble-averaged current and charge densities.

A model potential of the form $V(\vec{r}) = V(x,y) + V(z)$ is used to isolate contributions to the conductivity due to potential-broadened levels. The consequences of this model, for the wave functions and matrix elements, are discussed in Sec. V. In Sec. VI we examine the case of transverse conductivity for wave propagation parallel to $\vec{B}$. This geometry is important to helicon propagation and Doppler-shifted cyclotron resonance.[9] New expressions for a broadened-level magnetic-field-dependent effective mass and a finite-wavelength conductivity appropriate to transverse magnetoacoustic are obtained. These expressions are shown to oscillate as a function of $1/B$ where $B = |\vec{B}|$. The magnitudes of these quantities are discussed in Sec. VII.

II. EIGENFUNCTIONS AND EIGENVALUES

The important feature of the wave functions used here is their translational invariance. This invariance property arises because the wave functions are required to be simultaneous eigenfunctions of a commuting set of MTO. In general, the operators $\tau(\vec{R}_n)$ are noncommutative, but restricting the quantum of flux through a unit cell to be a *rational* multiple of 2π yields a commuting subset of MTO.[5,6] Although the details of the investigation are simplified by this restriction, the results are very general and apparently independent of the rationality assumption. We express this condition in the following way:

$$\vec{b} \equiv e\vec{B}/\hbar c = (2\pi s/N)\cdot(\vec{a}_3/\Delta)\,, \tag{2.1}$$

where s/N is a rational number and $\Delta = (\vec{a}_1 \times \vec{a}_2)\cdot\vec{a}_3$. We take N even. $\vec{a}_1, \vec{a}_2$, and $\vec{a}_3$ are primitive lattice vectors. For $\vec{b}$ satisfying Eq. (2.1), commuting subsets can be constructed. The subset we chose to work with has a typical element $\tau(n_1\vec{a}_1 + n_2N\vec{a}_2 + n_3\vec{a}_3)$. Here n_1, n_2, and n_3 are integers. One further restriction is imposed. We require all functions of interest to satisfy magnetic periodic boundary conditions[6]

$$\tau(N_i\vec{a}_i)f(\vec{r}) = f(\vec{r})\,, \quad i = 1, 2, 3 \tag{2.2}$$

where $N_i\vec{a}_i$ is a macroscopic length.

To determine the general properties of the wave functions, irreducible representations of the MTO are constructed. The wave functions are then required to span the representation matrices and we find that

$$\tau(\vec{R}_n)\psi(\vec{r}, n\vec{\kappa}\sigma) = \sum_{\sigma'} \Gamma^{\vec{\kappa}}_{\sigma',\sigma}(\vec{R}_n)\psi(\vec{r}, n\vec{\kappa}\sigma')\,, \tag{2.3}$$

where $\Gamma^{\vec{\kappa}}_{\sigma',\sigma}(\vec{R}_n)$ are the matrix elements. For an orthorhombic system (see Appendix A), we have

$$\Gamma^{\vec{\kappa}}_{\sigma',\sigma}(\vec{R}_n) = \exp\{i[\vec{\kappa} + (\sigma s/N)\vec{K}_1]\cdot(n_1'\vec{a}_1 + \vec{R}_N)\}$$
$$\times \exp[i(s/4\pi N)(\vec{K}_1\cdot\vec{R}_n)(\vec{K}_2\cdot\vec{R}_n)]$$
$$\times \exp[i\kappa_y a_2(\sigma + n_2' - \sigma')]\delta_{\sigma',\sigma+n_2}(\text{modulo } N), \tag{2.4}$$

where

$$\vec{\kappa} = \kappa_x\hat{x}_0 + \kappa_y\hat{y}_0 + \kappa_z\hat{z}_0; \qquad -\frac{\pi}{Na_1} \le \kappa_x < \frac{\pi}{Na_1}\,,$$
$$-\frac{\pi}{Na_2} \le \kappa_y < \frac{\pi}{Na_2}\,, \qquad -\frac{\pi}{a_3} \le \kappa_z < \frac{\pi}{a_3}\,;$$
$$a_i = |\vec{a}_i|\,, \qquad i = 1, 2, 3.$$

σ and σ' vary from 0 to $N-1$. $\vec{K}_i = \vec{a}_j \times \vec{a}_k/\Delta$ and cyclic permutations,

$$\vec{R}_N = n_1N\vec{a}_1 + n_2N\vec{a}_2 + n_3\vec{a}_3\,.$$

The primes on the integers n_1 and n_2 indicate that they are restricted to values less than N. The term modulo N means that whenever $n_2' + \sigma > N$, the Kronecker delta becomes $\delta_{\sigma',\sigma+n_2'-N}$.

Several interesting properties of the wave functions are available. First, wave functions satisfying Eq. (2.3) may be written in Bloch-like form:

$$\psi(\vec{r}\,; n\vec{\kappa}\sigma) = (\exp[i\,[\vec{\kappa} + (\sigma s/N)\vec{K}_1]\cdot\vec{r}\,])\,\mathcal{W}(\vec{r}\,; n\vec{\kappa}\sigma), \tag{2.5}$$

where

$$\tau(\vec{a}_1)\mathcal{W}(\vec{r}\,; n\vec{\kappa}\sigma) = \tau(N\vec{a}_2)\mathcal{W}(\vec{r}\,; n\vec{\kappa}\sigma)$$
$$= \tau(\vec{a}_3)\mathcal{W}(\vec{r}\,; n\vec{\kappa}\sigma) = \mathcal{W}(\vec{r}\,; n\vec{\kappa}\sigma). \tag{2.6}$$

Second, the eigenvalues of $\mathcal{H}_0$, $\epsilon(n, \vec{\kappa})$ are independent of σ. This result which is demonstrated in Appendix B indicates that each level is N-fold degenerate. A formal prescription for finding the eigenvalues is outlined in Appendix C.

From Eq. (2.1) we see that small changes in B result in discontinuous changes in the degeneracy of a system. However, the degeneracy is not an observable, and an examination of the density of states for fields restricted by Eq. (2.1) shows that small changes in B produce continuous changes in the density of states.[6,12]

Another feature of electron states having the properties expressed by Eqs. (2.5) and (2.6) is that the expectation value of the velocity operator equals

$$\frac{1}{\hbar}\frac{\partial\epsilon}{\partial\vec{\kappa}}(n, \vec{\kappa})\,.$$

More generally, as first indicated by Harper, the matrix element of the velocity operator $d\vec{r}/dt$ is[12]

$$\left\langle n'\vec{\kappa}'\sigma' \left| \frac{d\vec{r}}{dt} \right| n\vec{\kappa}\sigma \right\rangle = \delta_{\vec{\kappa}'\vec{\kappa}}\delta_{\sigma'\sigma}\left(\delta_{n'n}\frac{1}{\hbar}\frac{\partial\epsilon}{\partial\vec{\kappa}}(n,\vec{\kappa}) - \frac{i}{\hbar}\left[\epsilon(n'\vec{\kappa}) - \epsilon(n,\vec{\kappa})\right]\vec{R}(n'n,\vec{\kappa})\right), \tag{2.7}$$

where

$$\vec{R}(n'n,\vec{\kappa}) = \frac{\Omega}{N\Delta}\int_{\Delta'} d^3\vec{r}\; \mathcal{W}^*(\vec{r}; n'\vec{\kappa}0)\frac{\partial}{\partial\vec{\kappa}}\mathcal{W}(\vec{r}; n\vec{\kappa}0). \tag{2.8}$$

Ω denotes the volume of the periodicity domain and Δ' is the volume of a primitive magnetic unit cell $(\vec{a}_1\times N\vec{a}_2)\cdot\vec{a}_3$. The symbol $\langle\,|\,|\,\rangle$ denotes matrix integration over the periodicity domain. The form of the matrix element of the velocity operator is the same as for Bloch functions. The significant feature of this result as it applies to magnetic field problems is that the diagonal-matrix element for motion normal to the magnetic field is not zero. This result is a consequence of the broadening of the oscillator levels. In the free-electron case, only the off-diagonal elements are nonzero.

Another important result is the sum rule[1,12]

$$\frac{m}{\hbar^2}\frac{\partial^2\epsilon}{\partial\kappa_i\partial\kappa_j}(n,\vec{\kappa}) - \delta_{ij} = \sum_{n'\neq n}\left(\left\langle n\vec{\kappa}\sigma\left|\frac{dx_i}{dt}\right|n'\vec{\kappa}\sigma\right\rangle\left\langle n'\vec{\kappa}\sigma\left|\frac{dx_j}{dt}\right|n\vec{\kappa}\sigma\right\rangle + \left\langle n\vec{\kappa}\sigma\left|\frac{dx_j}{dt}\right|n'\vec{\kappa}\sigma\right\rangle\left\langle n'\vec{\kappa}\sigma\left|\frac{dx_i}{dt}\right|n\vec{\kappa}\sigma\right\rangle\right)\times[\epsilon(n,\vec{\kappa}) - \epsilon(n',\vec{\kappa})]^{-1}, \tag{2.9}$$

which will be used in the definition of a magnetic-field-dependent effective mass. Both Eqs. (2.7) and (2.9) will be used in interpreting the result of the transport calculations. We consider next a prescription for obtaining the magnetic-field-dependent transport coefficients.

III. DENSITY MATRIX

We consider a collection of N_e independent electrons in the periodicity domain subject to the Hamiltonian

$$\mathcal{H}_T = \mathcal{H}_0 + \mathcal{H}_1 + \mathcal{H}_2, \tag{3.1}$$

with

$$\mathcal{H}_1 = \frac{-e}{2mc}\left[\left(\vec{p} - \frac{e\vec{A}_0}{c}\right)\cdot\vec{A}_1(\vec{r},t) + \vec{A}_1(\vec{r},t)\cdot\left(\vec{p} - \frac{e\vec{A}_0}{c}\right)\right] + e\phi_1(r,t). \tag{3.2}$$

$\mathcal{H}_1$ describes the interaction of the electrons with the space- and time-dependent perturbations represented, respectively, by the vector and scalar potentials $\vec{A}_1(\vec{r},t)$ and $\phi_1(\vec{r},t)$. $\mathcal{H}_2$ denotes the electron interactions with thermal phonons, impurity scattering centers, etc.

The magnetotransport effects for electrons in the above environment are obtained by examining the ensemble-averaged current and charge densities for a single representative electron at position $\vec{r}_e$ and time t. The current and charge densities are, respectively,[10]

$$\vec{j}(\vec{r}_e,t) = \tfrac{1}{2}e\sum_{\nu,\nu'}\rho_{\nu\nu'}(t)\langle\nu'|\,\vec{v}\delta(\vec{r}-\vec{r}_e) + \delta(\vec{r}-\vec{r}_e)\vec{v}\,|\nu\rangle, \tag{3.3}$$

$$n(\vec{r}_e,t) = e\sum_{\nu,\nu'}\rho_{\nu\nu'}(t)\langle\nu'|\delta(\vec{r}-\vec{r}_e)|\nu\rangle, \tag{3.4}$$

with $\vec{v} = m^{-1}(\vec{p} - e\vec{A}_0/e - e\vec{A}_1/c)$. $\rho_{\nu\nu'}(t)$ is an element of the density matrix, and ν denotes the labeling of a magnetic eigenstate. The evaluation of the density matrix is carried out next. The elements of the density matrix satisfy the equation of motion:

$$i\hbar\frac{d}{dt}\rho_{\nu\nu'}(t) = \sum_{\nu''}\langle\nu|\mathcal{H}_T|\nu''\rangle\rho_{\nu''\nu'}(t) - \sum_{\nu''}\rho_{\nu\nu''}(t)\langle\nu''|\mathcal{H}_T|\nu'\rangle. \tag{3.5}$$

Equation (3.5) is simplified by treating the operator $\mathcal{H}_2$ by its effect of relaxing the density matrix to its instantaneous thermal equilibrium[13] value $\bar{\rho}_{\nu\nu'}(t)$:

$$\left(i\hbar\frac{d}{dt} + \epsilon(\nu') - \epsilon(\nu)\right)\rho_{\nu\nu'}(t) = \sum_{\nu''}(\langle\nu|\mathcal{H}_1|\nu''\rangle\rho_{\nu''\nu'}(t) - \rho_{\nu\nu''}(t)\langle\nu''|\mathcal{H}_1|\nu'\rangle) - \frac{i\hbar}{\tau_{\nu\nu'}}(\rho_{\nu\nu'}(t) - \bar{\rho}_{\nu\nu'}(t)), \tag{3.6}$$

where $\tau_{\nu\nu'}$ is a relaxation time. For Fermi statistics

$$\bar{\rho}_{\nu\nu'}(t) = (\tfrac{1}{2}N_e)^{-1} \times \langle \nu | \{1 + \exp[(\mathcal{H}_0 + \mathcal{H}_1 - \mu_0 - \mu_1(\vec{r}, t))/kT]\}^{-1} | \nu' \rangle. \tag{3.7}$$

Here μ_0 is the Fermi energy in the absence of the perturbations and $\mu_1(\vec{r}, t)$ is the change in the Fermi energy due to the perturbations; $\mu_1(\vec{r}, t)$ is unknown, k is Boltzmann's constant, and T is the absolute temperature

Equation (3.6) contains two unknowns, $\rho_{\nu\nu'}(t)$ and $\bar{\rho}_{\nu\nu'}(t)$. Another equation is needed. It is provided by the constraint that the ensemble-averaged time rate of change of particle density at $(\vec{r}_e, t)$ due to collisions is zero.[14] This is given by the equation

$$\sum_{\nu\nu'} \langle \nu' | \delta(\vec{r} - \vec{r}_e) | \nu \rangle (\rho_{\nu\nu'}(t) - \bar{\rho}_{\nu\nu'}(t))/\tau_{\nu\nu'} = 0 \ . \tag{3.8}$$

Equation (3.8) will be used later in the evaluation of $\mu_1(\vec{r}, t)$. Of immediate interest is Eq. (3.6), which we linearize. We first write

$$\begin{aligned} \rho_{\nu\nu'}(t) &= \rho_\nu^0 \delta_{\nu\nu'} + \rho_{\nu\nu'}^1(t) , \\ \bar{\rho}_{\nu\nu'}(t) &= \rho_\nu^0 \delta_{\nu\nu'} + \bar{\rho}_{\nu\nu'}^1(t) , \end{aligned} \tag{3.9}$$

where[10]

$$\rho_\nu^0 = (\tfrac{1}{2}N_e)^{-1}[1 + e^{(\epsilon(\nu) - \mu_0)/kT}]^{-1} , \tag{3.10}$$

$$\bar{\rho}_{\nu\nu'}^1(t) = \frac{\rho_{\nu'}^0 - \rho_\nu^0}{\epsilon(\nu') - \epsilon(\nu)} [\langle \nu | \mathcal{H}_1 | \nu' \rangle - \langle \nu | \mu_1(\vec{r}, t) | \nu' \rangle] .$$

The linearized equation of motion is then

$$\begin{aligned} i\hbar \left(\frac{d}{dt} + \frac{1}{\tau} \right) \rho_{\nu\nu'}^1 + [\epsilon(\nu') - \epsilon(\nu)] \rho_{\nu\nu'}^1 &= (\rho_{\nu'}^0 - \rho_\nu^0) \langle \nu | \mathcal{H}_1 | \nu' \rangle + \frac{i\hbar}{\tau} \frac{\rho_{\nu'}^0 - \rho_\nu^0}{\epsilon(\nu') - \epsilon(\nu)} \\ &\quad \times \langle \nu | \mathcal{H}_1 - \mu_1(\vec{r}, t) | \nu' \rangle . \end{aligned} \tag{3.11}$$

Equation (3.11) is solved subject to $\rho_{\nu\nu'}^1(t = -\infty) = 0$ with $\mathcal{H}_1$ slowly turned on. We have also taken the relaxation time to be independent of ν and ν'.

For real potentials equal to

$$\begin{aligned} \vec{A}_1(\vec{r}, t) &= e^{\alpha t}[A_1(\vec{q}, \omega) e^{i(\vec{q} \cdot \vec{r} - \omega t)} + \vec{A}_1(-\vec{q}, -\omega) e^{-i(\vec{q} \cdot \vec{r} - \omega t)}] , \\ \phi_1(\vec{r}, t) &= e^{\alpha t}[\phi_1(\vec{q}, \omega) e^{i(\vec{q} \cdot \vec{r} - \omega t)} + \phi_1(-\vec{q}, -\omega) e^{-i(\vec{q} \cdot \vec{r} - \omega t)}], \end{aligned} \tag{3.12}$$

where $e^{\alpha t}$ is a convergence factor, we find that

$$\begin{aligned} \rho_{\nu\nu'}^1(t) = e^{\alpha t} \frac{\rho_{\nu'}^0 - \rho_\nu^0}{\epsilon(\nu') - \epsilon(\nu)} & \left[\left(1 - \frac{\hbar\bar{\omega}}{\epsilon(\nu') - \epsilon(\nu) + \hbar\bar{\omega} + i\hbar/\tau} \right) \langle \nu | \mathcal{H}_1(\vec{q}, \omega) | \nu' \rangle e^{-i\omega t} \right. \\ & \left. + \left(1 + \frac{\hbar\bar{\omega}^*}{\epsilon(\nu') - \epsilon(\nu) - \hbar\bar{\omega}^* + i\hbar/\tau} \right) \langle \nu | \mathcal{H}_1(-\vec{q}, -\omega) | \nu' \rangle e^{i\omega t} \right] \\ & - \frac{i\hbar}{\tau} \frac{\rho_{\nu'}^0 - \rho_\nu^0}{\epsilon(\nu') - \epsilon(\nu)} \left(\sum_{\vec{q}', \omega'} \frac{\mu_1(\vec{q}', \omega') \langle \nu | e^{i\vec{q}' \cdot \vec{r}} | \nu' \rangle e^{-i\omega' t}}{\epsilon(\nu') - \epsilon(\nu) + \hbar\bar{\omega} + i\hbar/\tau} + \sum_{\vec{q}', \omega'} \frac{\mu_1(-q', -\omega') \langle \nu | e^{-i\vec{q}' \cdot \vec{r}} | \nu' \rangle e^{i\omega' t}}{\epsilon(\nu') - \epsilon(\nu) - \hbar\bar{\omega}^* + i\hbar/\tau} \right), \end{aligned} \tag{3.13}$$

where

$$\bar{\omega} = \omega + i\alpha, \quad \bar{\omega}' = \omega' + i\alpha$$

and

$$\mathcal{H}_1(\pm\vec{q}, \pm\omega) = -\frac{e}{c} \vec{V}(\pm\vec{q}) \cdot \vec{A}_1(\pm\vec{q}, \pm\omega) + e\phi_1(\pm\vec{q}, \pm\omega) e^{\pm i\vec{q} \cdot \vec{r}} , \tag{3.14}$$

$$\vec{V}(\pm\vec{q}) = \frac{1}{2m} \left[\left(\vec{p} - \frac{e\vec{A}_0}{c} \right) e^{\pm i\vec{q} \cdot \vec{r}} + e^{\pm i\vec{q} \cdot \vec{r}} \left(\vec{p} - \frac{e\vec{A}_0}{c} \right) \right] . \tag{3.15}$$

In the above we have Fourier analyzed $\mu_1(\vec{r}, t)$. We are now able to examine the current and chage densities.

IV. CURRENT AND CHARGE DENSITIES

The ensemble-averaged current and charge densities are given by Eqs. (3.3) and (3.4). We separate each equation into a part that is explicitly a time-independent part and a time-dependent part. Both parts are Fourier analyzed. The Fourier transform of the explicitly time-independent part of the current density is zero; for the charge density, it is $(e/\Omega)\delta\vec{q},0$. For the time-dependent parts, denoted by $\vec{j}_1(\vec{r}_e,t)$ and $n_1(\vec{r}_e,t)$, we write

$$[\vec{j}_1(\vec{r}_e,t);n_1(\vec{r}_e,t)=e^{\alpha t}\sum_{\vec{q},\omega}[\vec{j}_1(\vec{q},\omega);n_1(\vec{q},\omega)] \times e^{i(\vec{q}\cdot\vec{r}_e-\omega t)}+\text{c. c.}, \tag{4.1}$$

where $\vec{q}$ is restricted to the first Brillouin zone and

$$[\vec{j}_1(\vec{q},\omega);n_1(\vec{q},\omega)]=(2\pi\Omega)^{-1}\int dt\int d^3\vec{r}_e\,e^{-\alpha t} \times [\vec{j}_1(\vec{r}_e,t);n_1(\vec{r}_e,t)]e^{-i(\vec{q}\cdot\vec{r}_e-\omega t)}. \tag{4.2}$$

Using Eq. (3.13) and retaining terms linear in the fields, we obtain

$$\vec{j}_1(\vec{q},\omega)=\frac{e^2}{mc\Omega}\left[-[\overleftrightarrow{1}+\overleftrightarrow{1}(\vec{q},\bar{\omega})]\cdot\frac{E(\vec{q},\omega)}{i\bar{\omega}/c}+\frac{i\hbar}{\tau}\vec{C}(\vec{q},\bar{\omega})\left(\phi_1(\vec{q},\omega)-\frac{\mu_1}{e}(\vec{q},\omega)\right)\right], \tag{4.3}$$

$$n_1(\vec{q},\omega)=\frac{e^2}{mc^2\Omega}\left[-\vec{K}(\vec{q},\bar{\omega})\cdot\frac{E(\vec{q},\omega)}{i\bar{\omega}/c}+\frac{i\hbar}{\tau}\gamma(\vec{q},\bar{\omega})\left(\phi_1(\vec{q},\omega)-\frac{\mu_1}{e}(\vec{q},\omega)\right)\right], \tag{4.4}$$

where $\overleftrightarrow{1}$ is the unit dyadic and

$$\overleftrightarrow{1}(\vec{q},\bar{\omega})=m\sum_{\nu,\nu'}\frac{\rho^0_{\nu'}-\rho^0_\nu}{\epsilon(\nu')-\epsilon(\nu)}\left(1-\frac{\hbar\bar{\omega}}{\epsilon(\nu')-\epsilon(\nu)+\hbar\bar{\omega}+i\hbar/\tau}\right)\langle\nu|\vec{V}(-\vec{q})|\nu\rangle\langle\nu|\vec{V}(\vec{q})|\nu'\rangle, \tag{4.5}$$

$$\vec{K}(\vec{q},\bar{\omega})=mc\sum_{\nu,\nu'}\frac{\rho^0_{\nu'}-\rho^0_\nu}{\epsilon(\nu')-\epsilon(\nu)}\left(1-\frac{\hbar\bar{\omega}}{\epsilon(\nu')-\epsilon(\nu)+\hbar\bar{\omega}+i\hbar/\tau}\right)\langle\nu'|e^{-i\vec{q}\cdot\vec{r}}|\nu\rangle\langle\nu|\vec{V}(\vec{q})|\nu'\rangle, \tag{4.6}$$

$$\gamma(q,\bar{\omega})=mc^2\sum_{\nu,\nu'}\frac{\rho^0_{\nu'}-\rho^0_\nu}{\epsilon(\nu')-\epsilon(\nu)}\frac{|\langle\nu|e^{i\vec{q}\cdot\vec{r}}|\nu'\rangle|^2}{\epsilon(\nu')-\epsilon(\nu)+\hbar\bar{\omega}+i\hbar/\tau}, \tag{4.7}$$

and

$$\vec{C}(\vec{q},\omega)=\frac{\vec{K}(-\vec{q},0)-[\overleftrightarrow{1}+\overleftrightarrow{1}(\vec{q},\omega)]\cdot\vec{q}c/\bar{\omega}}{\hbar\bar{\omega}+i\hbar/\tau}. \tag{4.8}$$

In the above equation

$$\frac{\vec{E}(\vec{q},\omega)}{(i\bar{\omega}/c)}=\vec{A}_1(\vec{q},\omega)-\vec{q}\frac{c}{\bar{\omega}}\phi_1(\vec{q},\omega).$$

In arriving at these equations we have used the selection rule $\delta_{\vec{q}\vec{q}'}$ which is valid even though the restriction on $\vec{q}$ allows any two vectors to differ by a vector of type $\vec{\mathcal{K}}\equiv n_1\vec{K}_1/N+n_2\vec{K}_2/N+n_3\vec{K}_3$.[12]

To completely determine the current and charge densities we Fourier analyze Eq. (3.8). We obtain

$$\phi_1(\vec{q},\omega)-\frac{\mu_1(\vec{q},\omega)}{e}=\frac{[\vec{K}^*(-\vec{q},0)-\vec{K}(\vec{q},\bar{\omega})]\cdot\vec{E}(\vec{q},\omega)/(i\bar{\omega}/c)}{\vec{K}(\vec{q},\omega)\cdot\vec{q}c/\bar{\omega}+\hbar\bar{\omega}\gamma(\vec{q},\bar{\omega})}. \tag{4.9}$$

By examining Eqs. (4.3), (4.4), and (4.9) we see that the theory is gauge invariant. It is also demonstrable that these equations satisfy the equation of continuity.

A general expression for the current density $\vec{j}_1(\vec{q},\omega)$ is now available:

$$\vec{j}_1(\vec{q},\omega)=(e^2/im\bar{\omega}\Omega)\left(-[\overleftrightarrow{1}+\overleftrightarrow{1}(\vec{q},\bar{\omega})]+\frac{(i\hbar/\tau)\vec{C}(\vec{q},\bar{\omega})[\vec{K}^*(-\vec{q},0)-\vec{K}(\vec{q},\bar{\omega})]}{\vec{K}(\vec{q}\,\bar{\omega})\cdot\vec{q}c/\omega+\hbar\bar{\omega}\gamma(\vec{q},\bar{\omega})}\right)\cdot\vec{E}(\vec{q},\omega). \tag{4.10}$$

We note that

$$n_1(\vec{q},\omega)=\vec{q}\cdot\vec{j}_1(\vec{q},\omega)/\bar{\omega}.$$

To isolate the effects of potential broadening on the current, we evaluate Eq. (4.10) for a simplified model of the crystalline potential, where $V(x,y,z)=V(x,y)+V(z)$. The magnetic field is along the z axis.

V. MODEL

We write the Hamiltonian for the model potential as

$$\mathcal{H}_0 = \left[\frac{1}{2m}\left(\vec{p} - \frac{e\vec{A}_0}{c}\right)^2_\rho + V(\vec{\rho})\right] + \left(\frac{1}{2m}p_z^2 + V(z)\right) \tag{5.1}$$

or

$$\mathcal{H}_0 = \mathcal{H}_0(\vec{\rho}) + \mathcal{H}_0(z) \ , \tag{5.2}$$

where $\vec{\rho}$ is a position vector in the x-y plane. The eigenfunctions and energy eigenvalues are separable into

$$\psi(\vec{\rho}; n\vec{\kappa}_\rho\sigma)\eta(z; j\kappa_z)$$

and

$$\epsilon(nj, \vec{\kappa}) = \epsilon(n, \vec{\kappa}_\rho) + \epsilon(j, \kappa_z) \ ,$$

respectively, with the property

$$\mathcal{H}_0(\vec{\rho})\psi(\vec{\rho}; n\vec{\kappa}_\rho\sigma) = \epsilon(n, \vec{\kappa}_\rho)\psi(\vec{\rho}; n\vec{\kappa}_\rho\sigma) \ , \tag{5.3}$$

$$\mathcal{H}_0(z)\eta(z; j\kappa_z) = \epsilon(j, \kappa_z)\eta(z, j\kappa_z) \ , \tag{5.4}$$

where

$$\vec{\kappa}_\rho = \hat{x}_0\kappa_x + \hat{y}_0\kappa_y \ .$$

For

$$V(x, y) = V(-x, y) = V(x, -y)$$

and

$$V(z) = V(-z) \ ,$$

$$\epsilon(n, \kappa_x, \kappa_y) = \epsilon(n, -\kappa_x, \kappa_y) = \epsilon(n, \kappa_x, -\kappa_y)$$

and

$$\epsilon(j, \kappa_z) = \epsilon(j, -\kappa_z) \ .$$

We note that the index n is now associated *only* with motion in the x-y plane. In the limit of zero periodic potential, $\epsilon(n; \vec{\kappa}_\rho)$ is independent of $\vec{\kappa}_\rho$ and equal to $(n+\frac{1}{2})\hbar^2 b/m$, the energy of a Landau level ($b = |\vec{b}|$).

The matrix elements of the velocity operator for the separated potential are obtained by separating the integration over the x-y plane from that along the z axis. The former is denoted by curly brackets, the latter by round ones:

$$\left\langle n'j'\vec{\kappa}'\sigma' \left| \frac{d\vec{\rho}}{dt} \right| nj\vec{\kappa}\sigma \right\rangle = \left\{ n'\vec{\kappa}'_\rho\sigma' \left| \frac{d\vec{\rho}}{dt} \right| n\vec{\kappa}_\rho\sigma \right\} (j'\kappa'_z | j\kappa_z)$$

$$= \delta_{\kappa',\kappa}\delta_{\sigma',\sigma}\delta_{j',j}\left\{\frac{1}{\hbar}\frac{\partial}{\partial\vec{\kappa}_\rho}\epsilon(n; \vec{\kappa}_\rho)\delta_{n',n} - \frac{i}{\hbar}[\epsilon(n', \vec{\kappa}_\rho) - \epsilon(n, \vec{\kappa}_\rho)]\vec{R}_{n'n}(\vec{\kappa}_\rho)\right\} , \tag{5.5}$$

$$\left\langle n'j'\vec{\kappa}'\sigma' \left| \frac{dz}{dt} \right| nj\vec{\kappa}\sigma \right\rangle = \{n'\vec{\kappa}'_\rho\sigma' | n\vec{\kappa}_\rho\sigma\} \left(j'\kappa'_z \left| \frac{dz}{dt} \right| j\kappa_z \right)$$

$$= \delta_{\kappa',\kappa}\delta_{\sigma',\sigma}\delta_{n',n}\left\{\frac{1}{\hbar}\frac{\partial}{\partial\kappa_z}\epsilon(j; \kappa_z)\delta_{j',j} - \frac{i}{\hbar}[\epsilon(j', \kappa_z) - \epsilon(j, \kappa_z)]Z_{j'j}(\kappa_z)\right\} \ , \tag{5.6}$$

where

$$\vec{R}_{n'n}(\vec{\kappa}_\rho) = \frac{N_1N_2}{N}\int_{\vec{a}_1} dx \int_{\vec{a}_2} dy \times \mathcal{W}^*(\vec{\rho}; n'\vec{\kappa}_\rho 0)\frac{\partial}{\partial\vec{\kappa}_\rho}\mathcal{W}(\vec{\rho}; n\vec{\kappa}_\rho 0) \ , \tag{5.7}$$

$$Z_{j'j}(\kappa_z) = N_3\int_{\vec{a}_3} dz\, \mathcal{U}^*(z; j'\kappa_z)\frac{\partial}{\partial\kappa_z}\mathcal{U}(z; j\kappa_z) \ , \tag{5.8}$$

and

$$\mathcal{W}(\vec{\rho}, n\vec{\kappa}_\rho 0) = e^{-i\vec{\kappa}_\rho\cdot\vec{\rho}}\psi(\vec{\rho}, n\vec{\kappa}_\rho 0);$$

$$\mathcal{U}(z, j\kappa_z) = e^{-i\kappa_z z}\eta(z; j\kappa_z) \ .$$

$\vec{R}_{n'n}(\vec{\kappa}_\rho)$ has components $X_{n'n}$ and $Y_{n'n}$ in the x and y directions, respectively.

VI. TRANSPORT COEFFICIENTS

With the above simplification we examine the current density for shear-wave propagation parallel to the magnetic field. The wave vector $\vec{q}$ is parallel to $\vec{B}$; $\vec{q} = (0, 0, q_z)$. This orientation is appropriate to the case of Doppler-shifted cyclotron resonance, as well as helicon propagation. Although the interest is in effects due to broadened levels, the analysis is applicable to the zero periodic potential limit, where the free-electron results are recovered. Effects due to umklapp processes are not included.

We consider Eq. (4.10). For transverse propagation

$K_x(q_z, \bar{\omega}) = K_y(q_z, \bar{\omega}) = 0$.

Because of the symmetry of dx/dt and dy/dt the components $I_{zy}(q_z, \bar{\omega})$, $I_{xz}(q_z, \bar{\omega})$, $I_{yz}(q_z, \bar{\omega})$, $I_{yz}(q_z, \bar{\omega})$ are zero. We examine $I_{xx}(q_z, \bar{\omega})$ and $I_{xy}(q_z, \bar{\omega})$. For $I_{xx}(q_z, \bar{\omega})$ (hereafter, we take $\bar{\omega} = \omega$)

$$I_{xx}(q_z, \omega) = m \sum_{nj, j'; \kappa\sigma} \frac{\rho^0_{nj'\vec{\kappa}-\vec{q}} - \rho^0_{nj\vec{\kappa}}}{\epsilon(j', \kappa_z - q_z) - \epsilon(j, \kappa_z)} \left(1 - \frac{\hbar\omega}{\epsilon(j', \kappa_z - q_z) - \epsilon(j, \kappa_z) + \hbar\omega + i\hbar/\tau}\right)$$

$$\times \left| \left\{ n\vec{\kappa}_\rho\sigma \left| \frac{dx}{dt} \right| n\vec{\kappa}_\rho\sigma \right\} \right|^2 |(j'\kappa_z - q_z | j\kappa_z)|^2 + m \sum_{n, n' \neq n; jj' \kappa\sigma} \frac{\rho^0_{n'j'\vec{\kappa}-\vec{q}} - \rho^0_{nj\vec{\kappa}}}{\epsilon(n'j', \vec{\kappa} - \vec{q}) - \epsilon(nj, \vec{\kappa})}$$

$$\times \left(1 - \frac{\hbar\omega}{\epsilon(n'j', \vec{\kappa} - \vec{q}) - \epsilon(nj, \vec{\kappa}) + \hbar\omega + i\hbar/\tau}\right) \left| \left\{ n'\kappa_\rho\sigma \left| \frac{dx}{dt} \right| n\vec{\kappa}_\rho\sigma \right\} \right|^2 |(j'\kappa_z - q_z | j\kappa_z)|^2 . \quad (6.1)$$

The first term in Eq. (6.1) contains elements for $n' = n$, the second term for $n' \neq n$. In the limit of zero periodic potential the first term of Eq. (6.1) is zero and the second reduces to Eq. (25) of Ref. 10 (with minor notational differences). In this limit the first term is zero because the expectation value of dx/dt is zero. For a finite periodic potential this term is not necessarily zero. $I_{xx}(q_z, \omega)$ is first examined in the limit of zero q_z.

In the limit as q_z approaches zero, $I_{xx}(q_z, \omega)$ is expressed as a power series in q_z with the first nonzero-q_z-dependent term being quadratic in q_z. The q_z-independent term contributes to the xx component of the conductivity tensor, an amount equal to

$$\sigma_{xx}(\omega) = ie^2 \lim_{q_z \to 0} \frac{(1 + I_{xx}(q_z, \omega))}{m\omega\Omega} ,$$

$$\sigma_{xx}(\omega) = \frac{e^2}{m\Omega} \frac{\tau}{1 - i\omega\tau} \frac{m}{\hbar^2} \sum_{nj\vec{\kappa}\sigma} \rho^0_{nj\vec{\kappa}} \frac{\partial^2\epsilon}{\partial\kappa_x^2} (n, \vec{\kappa}_\rho)$$

$$+ \frac{e^2}{\Omega\tau} (1 - i\omega\tau) \sum_{nj\vec{\kappa}\sigma} \rho^0_{nj\vec{\kappa}} \sum_{n' \neq n} X_{nn'} X_{n'n}$$

$$\times [(\epsilon(n, \vec{\kappa}_\rho) - \epsilon(n', \vec{\kappa}_\rho) + \hbar\omega + i\hbar/\tau)^{-1}$$

$$+ (\epsilon(n, \vec{\kappa}_\rho) - \epsilon(n', \vec{\kappa}_\rho) - \hbar\omega - i\hbar/\tau)^{-1}] . \quad (6.2)$$

The significant result here is the first term. This term is zero for zero periodic potential and finite for finite potential. It describes the response of a particle of mass

$$M^{-1}_{xx} = \frac{1}{\hbar^2} \sum_{nj\vec{\kappa}\sigma} \rho^0_{nj\vec{\kappa}} \frac{\partial^2\epsilon}{\partial\kappa_x^2} (n, \vec{\kappa}_\rho) \quad (6.3)$$

to an rf field of frequency ω. The finite value of M^{-1}_{xx} arises strictly from the infinite width of the magnetic band. Free-electron Landau levels are infinitesimally small and lead to an infinite magnetic-field-dependent effective mass. If the periodic potential serves only to broaden the Landau level while still maintaining the integrity of each Landau energy level, then the major contribution to M_{xx} occurs when a broadened level crosses the Fermi surface. For this case, oscillations of M_{xx} that are periodic in B^{-1} occur. An estimate of this effect is made in Sec. VII.

The second part of Eq. (6.2) can be interpreted with semiclassical concepts. This term indicates a true resonance for

$$\epsilon(n', \vec{\kappa}_\rho) - \epsilon(n, \vec{\kappa}_\rho) = \pm \hbar\omega.$$

When this condition is satisfied a series of peaks in the conductivity occur. In the zero potential limit where only adjacent Landau levels are coupled, one peak occurs. For zero potential and the classical limit, $\sigma_{xx}(\omega)$ reduces to

$$\sigma^{(\omega)}_{xx} = \frac{e^2\tau}{m\Omega} \left[\frac{1 - i\omega\tau}{1 + (\hbar^2 b^2/m^2 - \omega^2)\tau^2 - 2i\omega\tau} \right] . \quad (6.4)$$

Consider

$$I_{xy}(q_z, \omega) = m \sum_{n, n' \neq n; j, j' \vec{\kappa}\sigma} \frac{\rho^0_{n'j'\vec{\kappa}-\vec{q}} - \rho^0_{nj\vec{\kappa}}}{\epsilon(n'j', \vec{\kappa} - \vec{q}) - \epsilon(nj, \vec{\kappa})} |(j\kappa_z | j'\kappa_z - q_z)|^2$$

$$\times \left(1 - \frac{\hbar\omega}{\epsilon(n'j', \vec{\kappa} - \vec{q}) - \epsilon(nj, \vec{\kappa}) + \hbar\omega + i\hbar/\tau}\right) \left\{ n'\vec{\kappa}_\rho\sigma \left| \frac{dx}{dt} \right| n\vec{\kappa}_\rho\sigma \right\} \left\{ n\vec{\kappa}_\rho\sigma \left| \frac{dy}{dt} \right| n'\vec{\kappa}_\rho\sigma \right\} . \quad (6.5)$$

We first examine $I_{xy}(q_z, \omega)$ in the limit of zero q_z. In this limit the q_z-independent term contributes an amount to the xy component of the conductivity

$$\sigma_{xy}(\omega) = ie^2 \lim_{q_z \to 0} [1 + I_{xy}(q_z, \omega)]/m\omega\Omega ,$$

equal to

$$\sigma_{xy}(\omega) = \frac{-e^2}{m\Omega i\omega}\left(\frac{m\omega}{\hbar}\sum_{nj\vec{\kappa}\sigma}\rho^0_{nj\kappa}\sum_{n'\neq n} X_{nn'}X_{n'n} - Y_{nn'}Y_{n'n} - \frac{im\omega}{\tau}(1 - i\omega\tau)\right.$$

$$\left.\times \sum_{nj\kappa\sigma}\rho^0_{nj\kappa}\sum_{n'\neq n}\frac{X_{nn'}Y_{n'n}}{\epsilon(n,\vec{\kappa}_\rho) - \epsilon(n',\vec{\kappa}_\rho) + \hbar\omega + i\hbar/\tau} + \frac{Y_{nn'}X_{n'n}}{\epsilon(n,\vec{\kappa}_\rho) - \epsilon(n',\vec{\kappa}_\rho) - \hbar\omega - i\hbar/\tau}\right) . \qquad (6.6)$$

Here because of the assumed symmetry of the crystalline potential no term can be identified as the xy component of a magnetic-field-dependent effective mass. $\sigma_{xy}(\omega)$ yields results that are semiclassical in compostion. In the classical limit we get

$$\sigma_{xy} = \frac{e^2\tau}{m\Omega}\;\frac{\hbar b\tau/m}{1 + (\hbar^2 b^2/m^2 - \omega^2)\tau^2 - 2i\omega\tau} . \qquad (6.7)$$

We next consider the conductivity for finite q_z. We separate the current density $\vec{j}_1(q_z, \omega)$ into two parts, one without and one with frequency-dependent coefficients. The part with frequency-independent coefficients is

$$\vec{J}_M = -\frac{e^2}{mc\Omega}[\overleftrightarrow{1} + \overleftrightarrow{I}(q_z, 0)] \cdot \left(\vec{A}_1(q_z, \omega) + \vec{q}\frac{e}{\omega}\phi_1(q_z, \omega)\right), \qquad (6.8)$$

and is identified as a magnetization current. This can be seen by choosing the gauge $\phi_1(q_z, \omega) = 0$ and going to the limit $\omega = 0$, where there is no electric field. In Eq. (6.8) $\overleftrightarrow{I}(q_z, 0)$ is obtained from $\overleftrightarrow{I}(q_z, w)$ by setting $\omega = 0$.

The frequency-dependent part of $\vec{j}_1(q_z, \omega)$ is denoted by $\vec{j}'(q_z, \omega)$, where

$$\vec{j}'(q_z, \omega) \equiv \overleftrightarrow{\sigma}'(q_z, \omega) \cdot \vec{E}(q_z, \omega) . \qquad (6.9)$$

We examine $\overleftrightarrow{\sigma}'(q_z, \omega)$, treating the electrons as free along the z axis. To describe the motion in the z direction, we combine the band index j and the wave number κ_z into the wave number k_z which varies from minus to plus infinity. From Eqs. (6.1) and (6.5), and the definition of $\overleftrightarrow{\sigma}'(q_z, \omega)$, we find that

$$\sigma'_{xx}(q_z, \omega) = \frac{e^2\tau}{\Omega}\frac{1}{\hbar^2}\sum_{n\vec{\kappa}_\rho\sigma k_z}\rho^0_{n\vec{\kappa}_\rho k_z}\frac{\partial^2\epsilon(n,\vec{\kappa}_\rho)}{\partial\kappa_x^2}\left[1 + i\tau\left(\frac{\hbar q_z}{m}k_z - \omega\right)\right]^{-1}$$

$$+ \frac{e^2\hbar}{i\Omega}\sum_{n,n'\neq n;\vec{\kappa}_\rho k_z\sigma}\frac{\rho^0_{n'\vec{\kappa}_\rho k_z - q_z} - \rho^0_{n\vec{\kappa}_\rho k_z}}{[\epsilon(n',\vec{\kappa}_\rho, k_z - q_z) - \epsilon(n,\vec{\kappa}_\rho, k_z)]}\;\frac{|\{n'\vec{\kappa}_\rho\sigma|dx/dt|n\vec{\kappa}_\rho\sigma\}|^2}{[\epsilon(n',\vec{\kappa}_\rho, k_z - q_z) - \epsilon(n,\vec{\kappa}_\rho, k_z) + \hbar\omega + i\hbar/\tau]}$$

$$\equiv \sigma^1_{xx}(q_z, \omega) + \sigma^2_{xx}(q_z, \omega) , \qquad (6.10)$$

and

$$\sigma'_{xy}(q_z, \omega) = \frac{e^2\hbar}{i\Omega}\sum_{n_\rho\vec{\kappa}\sigma k_z}\frac{\rho^0_{n'\vec{\kappa}_\rho k_z} - q_z\rho^0_{n\vec{\kappa}_\rho k_z}}{\epsilon(n',\vec{\kappa}_\rho, k_z - q_z) - \epsilon(n\vec{\kappa}_\rho, k_z)}\;\frac{\{n'\vec{\kappa}_\rho\sigma|dx/dt|n\vec{\kappa}_\rho\sigma\}\{n\vec{\kappa}_\rho\sigma|dy/dt|n'\vec{\kappa}_\rho\sigma\}}{\epsilon(n',\vec{\kappa}_\rho,k_z - q_z) - \epsilon(n,\vec{\kappa}_\rho,k_z) + \hbar\omega + i\hbar\tau} . \qquad (6.11)$$

$\sigma^1_{xx}(q_z, \omega)$ and $\sigma^2_{xx}(q_z, \omega)$ denote, respectively, the contributions from the first and second part of Eq. (6.10). The important result here is the term $\sigma^1_{xx}(q_z, \omega)$. The other terms are interpretable in terms of semiclassical concepts. The form of σ^1_{xx} is the same as the zero magnetic field conductivity of a particle in an electric field of frequency ω and wave vector q_z.[15] Contributions to this term arise because of the *finite* width of the broadened magnetic band. The analysis of this case is similar to that for the magnetic-field-dependent effective mass [Eq. (6.3)]. For the situation when the potential broadens the Landau levels, oscillations periodic in B^{-1} occur. For magnetoacoustics, simplifications arise when the condition $q_z\Lambda \gg 1$ is satisfied. Λ is the electron mean free path. In this case the significant contribution to $\sigma^1(q_z, \omega)$ comes from that region of the Fermi surface where $k_z \approx 0$ and when the Fermi surface lies within a broadened level. For this case information about the widths of isolated broadened bands is available. The details of this effect and a numerical estimate are given in Sec. VII.

Equations (6.10) and (6.11) can be placed into a simple form when the periodic potential possesses fourfold symmetry:

$$j^{\pm}(qz,\omega) = (e^2\tau/m\Omega)\, G^{\pm}(q_z, \omega)\, E^{\pm}(q_z, \omega) + \sigma^1_{xx}(q_z\omega)\, E^{\pm}(q_z, \omega) \quad , \tag{6.12}$$

with

$$[j^{\pm}(q_z, \omega); E^{\pm}(q_z, \omega)] = [j_x'(q_z, \omega) \pm i j_y'(q_z, \omega); E_x(q_z, \omega) \pm iE_y(q_z, \omega)] \quad , \tag{6.13}$$

$$G^{\pm}(q_z, \omega) = \frac{\sigma^2_{xx}(q_z, \omega) \mp i\sigma'_{xy}(q_z, \omega)}{e^2\tau/m\Omega} \quad . \tag{6.14}$$

In the limit of zero periodic potential $G^{\pm}(q_z, \omega)$ reduces to[9]

$$G^{\pm}(q_z, \omega) = \tfrac{3}{4}\int_{-1}^{+1} \frac{d\xi\,(1-\xi^2)}{1 + i\tau(q_z v_f \xi \pm \hbar b/m - \omega)} \quad , \tag{6.15}$$

where ξ is a dimensionless variable and v_f is the velocity of an electron at the Fermi surface. Equation (6.15) is obtained by neglecting effects associated with the discrete nature of the eigenvalue spectra and leads to the absorption edge associated with Doppler-shifted cyclotron resonance.

VII. NUMERICAL ESTIMATE

In this section we estimate M_{xx} and $\sigma^1_{xx}(q_z, \omega)$. We treat the electrons as free along the z axis and assume the periodic potential has fourfold symmetry about this axis. We let $V(x, y) = V(x) + V(y)$ and regard the potential as a perturbation on the empty-lattice eigenstates. These states are described by simultaneous eigenfunctions of the MTO and $\mathcal{H}_0$ in the limit of zero crystalline potential. We also set the integers s/N to $1/N$ [see Eq. (2.1)]. The empty-lattice eigenfunctions for this case are

$$\phi(\vec{r}, n\vec{\kappa}_\rho k_z\sigma) = e^{ik_z z} e^{ibxy/2} \sum_{m=-\infty}^{+\infty} e^{-imNa\kappa_y} \times e^{i(\kappa_x + 2\pi\sigma/Na + 2\pi m/a)x}\, v_n\left(\frac{\kappa_x + 2\pi\sigma/Na}{b} + y + mNa\right), \tag{7.1}$$

with

$$v_n(y) = (\Omega)^{-1/2}\left(\frac{Nab^{1/2}}{2^n n!\,\pi^{1/2}}\right)^{1/2} e^{-by^2/2} H_n(b^{1/2}q) . \tag{7.2}$$

H_n is a Hermite polynomial[16] of order n. n is the Landau level quantum number and is either a positive integer or zero. (A more general empty-lattice eigenfunction is used in Appendix A.) Using perturbation theory, we examine the situation when the width of the broadened level is less than the Landau level separation. To first order the energy of a broadened Landau level is

$$\epsilon(n, \vec{\kappa}_p, k_z) = \frac{\hbar^2 b}{m}\,(n+\tfrac{1}{2}) + \frac{\hbar^2 k_z^2}{2m} + V_n(\cos\kappa_x Na + \cos\kappa_y Na) \quad , \tag{7.3}$$

where

$$V_n = V_1 \int_{-\infty}^{+\infty} d\xi\, v_n[b^{-1/2}(\xi + Nab^{1/2})]\, v_n(b^{-1/2}\xi) \quad , \tag{7.4}$$

ξ is a dimensionless variable, and V_1 is the first Fourier coefficient in the Fourier expansion of the periodic potential. In terms of $\epsilon(n, \vec{\kappa}_p, k_z)$, we write M_{xx} [(Eq. (6.3)] as

$$1/M_{xx} = \textstyle\sum_n 1/M^n_{xx} \quad , \tag{7.5}$$

with

$$\frac{1}{M^n_{xx}} = \frac{-2N}{N_e}\frac{(Na)^2}{\hbar^2}\, V_n \sum_{\vec{\kappa}_\rho k_z}{}' \cos\kappa_x Na \quad , \tag{7.6}$$

where the prime denotes summation over occupied states. In Fig. 1 we sketch M^{-1}_{xx} as a function of B^{-1} for the case when only the first few broadened levels contribute.

To interpret Fig. 1, we examine Fig. 2. From Fig. 2 we see that there are values of k_z, k_1, for example, chosen such that for all κ_x and κ_y, $\epsilon(n, \vec{\kappa}_\rho, k_z) < \mu_0$ (μ_0 is the Fermi energy). For $k_z = k_1$ all states below μ_0 are fully occupied and a sum over κ_x and κ_y yields a zero result. For other values of k_z, k_2, for example, chosen so that there are values of κ_x and κ_y for which $\epsilon(n, \vec{\kappa}_\rho, k_z) = \mu_0$, the nth level is partially filled and a sum over κ_x and κ_y yields a nonzero result. Thus, contributions to Eq. (7.6) came only from partially filled bands. To estimate this result, we change the sum in Eq. (7.6) to an integral letting

$$\sum_{\vec{\kappa}_\rho k_z} \to (\Omega/8\pi^3)\int d\kappa_x d\kappa_y dk_z \quad . \tag{7.7}$$

Integrating over k_z, the sum in Eq. (7.6) becomes

$$-\frac{\Omega}{8\pi^3}\frac{(2m)^{1/2}}{\hbar} V_n \times\int \frac{d\kappa_x d\kappa_y \cos\kappa_x Na(\cos\kappa_x Na + \cos\kappa_y Na)}{[\mu_0 - (n+\frac{1}{2})\hbar^2 b/m]^{1/2}} \quad . \tag{7.8}$$

This expression is valid for $\mu_0 - (n+\frac{1}{2})\hbar^2 b/m \gg 2V_n$.

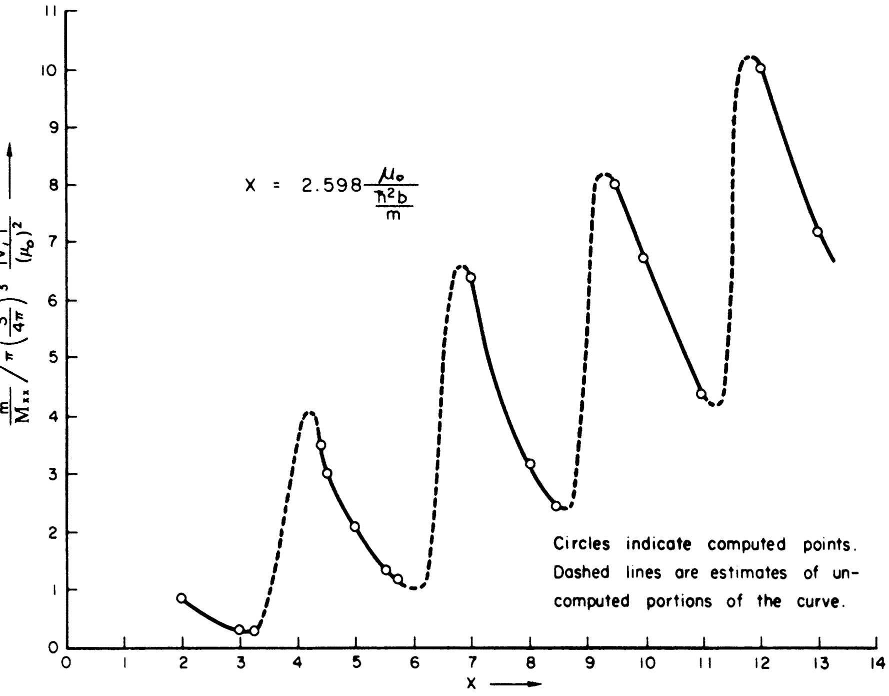

FIG. 1. Dependence of M_{xx}^{-1} on inverse magnetic field.

Integrating over κ_x and κ_y, we obtain

$$\frac{1}{M_{xx}^n} = \frac{1}{m}\,\frac{3\pi N}{4}\,\frac{V_n^2}{\mu_0^{3/2}[\mu_0 - (n+\frac{1}{2})\hbar^2 b/m]^{1/2}} \tag{7.9}$$

and

$$\frac{1}{M_{xx}} = \frac{1}{m}\,\frac{3\pi N}{4\mu_0^{3/2}}\sum_n \frac{V_n^2}{[\mu_0 - (n+\frac{1}{2})\hbar^2 b/m]^{1/2}} \;. \tag{7.10}$$

The computed points in Fig. 1 are obtained from Eq. (7.10).

Oscillations in the effective mass occur because as the magnetic field decreases, additional Landau levels cross the Fermi surface. This increases substantially the number of states contributing to M_{xx}^{-1}. As seen in Fig. 1, these oscillations are periodic in B^{-1}.

The above results were obtained for the situation when only the first few broadened Landau levels contributed. At more moderate magnetic fields higher Landau levels become important and most of the contributions to M_{xx} come from terms for which the integral in Eq. (7.4) has the asymptotic expansion[17]

$$\frac{(-1)^n \sin[n(2\phi - \sin 2\phi) + \frac{1}{4}\pi]}{(\pi \sin\phi)^{1/2}(\pi N n)^{1/4}}; \quad \pi N = 4n\cos^2\phi. \tag{7.11}$$

In this regime contributions from adjacent Landau levels are comparable and the oscillations decrease in amplitude and broaden as the magnetic field decreases. In this regime additional oscillations appear in M_{xx}^{-1} resulting from the term

$$\sin^2[n(2\phi - \sin 2\phi) + \tfrac{1}{2}\pi]\;. \tag{7.12}$$

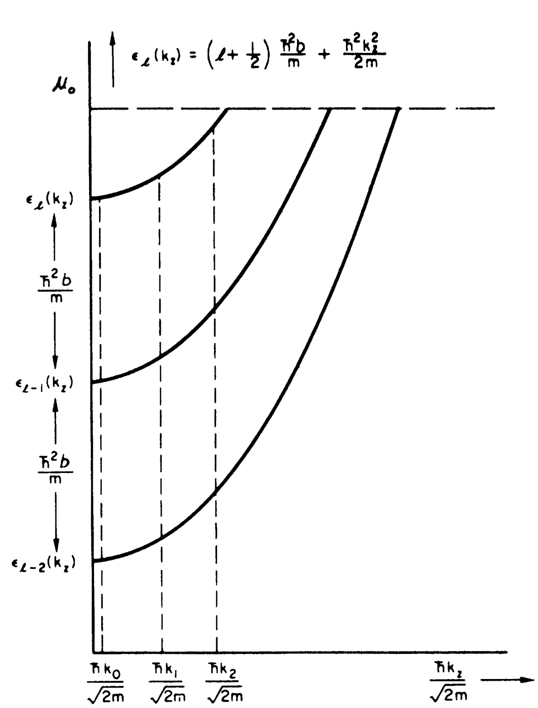

FIG. 2. Energy of a free electron in a magnetic field as a function of k_z.

This oscillatory behavior is generally expected to be of smaller amplitude and is related to the periodic variation in the level broadening of magnetic energy levels first discussed by Pippard.[18]

We now estimate the finite-wavelength conductivity coefficients important in magnetoacoustics and consider $\sigma^1_{xx}(q_z, \omega)$ [Eq. (6.10)] which for our approximation is

$$\sigma^1_{xx}(q_z,\omega) = -\frac{e^2\tau}{\Omega}\frac{(Na)^2}{\hbar^2} \times \sum_{n\bar{\kappa}_\rho k_z\sigma} o^0_{n\bar{\kappa}_\rho k_z} \frac{V_n \cos\kappa_x Na}{1+i\tau[(\hbar q_z/m)k_z-\omega]} . \quad (7.13)$$

We change the sum over $\kappa_x\kappa_y k_z$ into an integration and let $\kappa_x Na=\theta$, $\kappa_y Na=\varphi$, and $k_z = k_f\xi$:

$$\sigma^1_{xx}(q_z,\omega) = -\sigma_0\frac{3}{2(6\pi^2)^{2/3}}\sum_n \frac{V_n}{\hbar^2 b/m} \times \int' \frac{d\theta\, d\varphi\, d\xi \cos\theta}{1+i(q_z\Lambda\xi-\omega\tau)} . \quad (7.14)$$

The sum and integration are over occupied states. The symbols are

$$\Lambda = \frac{\hbar k_f \tau}{m}, \quad \sigma_0 = \frac{e^2\tau}{m\Omega}, \quad k_f = \left(\frac{2\mu_0}{\hbar^2}\right)^{1/2} .$$

We examine the real part of $\sigma^1_{xx}(q_z,\omega)$ for the situation $q_z\Lambda \gg 1$, where the denominator has a strong minimum at $\xi_0 \equiv \omega\tau/q_z\Lambda$. For the real part of $\sigma^1_{xx}(q_z,\omega)$, the reciprocal denominator is treated as Dirac delta-like function of constant area $\pi/q_z\Lambda$ centered at ξ_0:

$$\mathrm{Re}\,\sigma^1_{xx}(q_z,\omega) = -\sigma_0\frac{3}{2}\frac{1}{(6\pi^2)^{2/3}}\frac{\pi}{q_z\Lambda} \times \sum_n \frac{V_n}{\hbar^2 b/m}\int'_{\xi=\xi_0} d\theta\, d\varphi \cos\theta . \quad (7.15)$$

For metals, $\xi_0 \ll 1$. Thus, the important value of k_z is $k_z \approx 0$.

Here, as in the estimate of M_{xx}, contributions to the sum come only from partially filled bands. Unlike the previous estimate which included a sum over different values of k_z, here the only important value of k_z is $k_z = 0$. Further, the only important Landau level is the one for which $\epsilon(n,\kappa_\rho,0)=\mu_0$. For the case when the ratio of the broadening to the Landau level spacing is small, all bands (at $k_z=0$) except the one at the Fermi surface are fully occupied. Hence

$$|\mathrm{Re}\,\sigma^1_{xx}(q_z,\omega)| = \frac{3\pi}{4q_z\Lambda}\sigma_0\left(\frac{128}{9\pi}\right)^{1/3}\frac{V_{\bar{n}}}{\hbar^2 b/m}\beta_{\bar{n}} , \quad (7.16)$$

where $\bar{n}$ is the value of the Landau level at the Fermi surface. The quantity $\beta_{\bar{n}}$ is a number between 0 and 1 and is dependent on the position of the Fermi surface. The amplitude of $\mathrm{Re}\,\sigma^1_{xx}$ is proportional to the ratio $V_{\bar{n}}/(\hbar^2 b/m)$ of the broadening as given by perturbation theory to the Landau level spacing. The factor $3\pi\sigma_0/4q_z\Lambda$ is the amplitude of the semiclassical expression $\mathrm{Re}\,\sigma_0 G_\pm$[9] evaluated in the limit of large $q\Lambda$. The important point is that the amplitude of $\mathrm{Re}\,\sigma^1_{xx}$ is a direct measure of the width of the broadened band. Furthermore, since the effect occurs only for values of magnetic field such that the Fermi level falls within the broadened band, increments in the conductivity that are periodic in B^{-1} will occur. For Doppler-shifted cyclotron resonance experiments, this effect should occur beyond the absorbtion edge. These increments in the conductivity will manifest themselves as periodic changes in the sound-wave attenuation.

ACKNOWLEDGMENTS

The authors are grateful for stimulating discussions with George Persky and Mark Power.

APPENDIX A

In this Appendix we construct the representations of the MTO. Using the notation of Sec. II we consider an $(s/N)\times N_1N_2$-fold degenerate level of the empty-lattice Hamiltonian, where

$$\frac{1}{2m}\left(\vec{p}-\frac{e\vec{A}_0}{c}\right)^2 \phi(\vec{r}; nj\lambda, \vec{\kappa}\sigma) = \left[(n+\tfrac{1}{2})\frac{\hbar^2 b}{m} + \frac{\hbar^2}{2m}\left(\kappa_z + \frac{2\pi}{a_3}j\right)^2\right]\phi(r; nj\lambda, \vec{\kappa}\sigma) . \quad (A1)$$

The eigenfunctions $\phi(\vec{r}; nj\lambda, \vec{\kappa}\sigma)$ are symmetrized eigenfunctions of the commuting set of magnetic translation operators

$$\phi(r; nj\lambda, \kappa\sigma) = e^{ibxy/2}\, e^{i(\kappa_z + 2\pi j/a_3)z}\sum_{m=-\infty}^{+\infty}\exp\left[-im\left(\kappa_y\frac{Na_2}{s}+\frac{2\pi\lambda}{s}\right)\right] \times \exp\left[i\left(\kappa_x + \frac{2\pi s}{N}\frac{\sigma}{a_1}+\frac{2\pi m}{a_1}\right)x\right] v_n\left(\frac{\kappa_x + 2\pi s\sigma/Na_1}{b} + y + m\frac{nA_2}{s}\right) , \quad (A2)$$

with

$$v_n(y)=\frac{1}{\Omega}\left(\frac{Na_2/s}{2^n n!}\,\frac{b^{1/2}}{\pi^{1/2}}\right)^{1/2}\exp(-\tfrac{1}{2}by^2)\,H_n(b^{1/2}y)\ , \tag{A3}$$

$\lambda=0, 1, 2\ldots,\ s-1$, and j is an integer varying from plus to minus infinity. The functions $\phi(\vec{r};\,nj\lambda,\,\vec{\kappa}\sigma)$ constitute a complete orthonormal set over the periodicity domain Ω.

Matrix representations of the MTO are obtained by requiring the functions $\phi(\vec{r};\,nj\lambda,\,\vec{\kappa}\sigma)$ to form a basis for the matrices:

$$\tau(\vec{R}_n)\,\phi(\vec{r};\,nj\lambda,\,\vec{\kappa}\sigma)=\sum_{\sigma',\lambda';\vec{\kappa}_\rho'}\Gamma_{\sigma',\sigma;\vec{\kappa}_\rho',\vec{\kappa}_\rho\lambda',\lambda;}(\vec{R}_n)\,\phi(\vec{r},\,nj\lambda',\vec{\kappa}'\sigma')\delta_{\kappa_z'\kappa_z}\ , \tag{A4}$$

$$\Gamma_{\sigma',\sigma;\vec{\kappa}_\rho',\vec{\kappa}_\rho;\lambda',\lambda}(\vec{R}_n)=\int_\Omega d^3r\ \phi^*(\vec{r};\,nj\lambda',\vec{\kappa}'\sigma')\,\tau(\vec{R}_n)\,\phi(\vec{r};\,nj\lambda,\,\vec{\kappa}\sigma)\,\delta_{\kappa_z',\kappa_z}\ , \tag{A5}$$

or

$$\Gamma_{\sigma',\sigma;\vec{\kappa}_\rho',\vec{\kappa}_\rho;\lambda',\lambda}(\vec{R}_n)=\delta_{\vec{\kappa}_\rho'\vec{\kappa}_\rho}\,\delta_{\lambda'\lambda}\,\Gamma^{\vec{\kappa}}_{\sigma',\sigma}(\vec{R}_n)\ . \tag{A6}$$

$\Gamma^{\vec{\kappa}}_{\sigma',\sigma}(\vec{R}_n)$ is given by Eq. (2.4). It is demonstrable that the matrix $\Gamma^{\vec{\kappa}}(\vec{R}_n)$ with elements $\Gamma^{\vec{\kappa}}_{\sigma',\sigma}(\vec{R}_n)$ is a representation of the MTO.[12] The matrices $\Gamma^{\vec{\kappa}}(\vec{R}_n)$ are irreducible.

Consider next the set of matricies

$$\mathfrak{D}^{\vec{\kappa}}=\{\Gamma^{\vec{\kappa}}(\vec{R}_1),\ \Gamma^{\vec{\kappa}}(\vec{R}_2),\ \ldots,\ \Gamma^{\vec{\kappa}}(\vec{R}_{N_1N_2N_3})\}\ . \tag{A7}$$

The $N_1N_2N_3/N^2$ different sets of $\mathfrak{D}^{\vec{\kappa}}$ obtained by varying $\vec{\kappa}$ over its designated range constitute all the inequivalent irreducible representations of the MTO.[12] The matrix elements satisfy the orthognality relation[12]

$$\sum_{\vec{R}_n}\Gamma^{\vec{\kappa}'*}_{\sigma,\sigma'}(\vec{R}_n)\,\Gamma^{\vec{\kappa}}_{\sigma'',\sigma'''}(\vec{R}_n)=\frac{N_1N_2N_3}{N}\,\delta_{\vec{\kappa}',\vec{\kappa}}\delta_{\sigma,\sigma''}\,\delta_{\sigma',\sigma'''}\ . \tag{A8}$$

APPENDIX B

In this Appendix, we demonstrate that the eigenvalues of $\mathcal{H}_0$ are independent of σ. Consider the matrix element

$$\langle n'\vec{\kappa}'\sigma'|\mathcal{H}_0|n\vec{\kappa}\sigma\rangle=\int_\Omega d^3x\,\psi^*(\vec{r};\,n'\vec{\kappa}'\sigma')\,\mathcal{H}_0\,\psi(\vec{r};\,n\vec{\kappa}\sigma)$$
$$=\int_\Omega d^3x\,[\tau(\vec{R}_n)\,\psi(\vec{r},\,n'\vec{\kappa}'\sigma')]^*$$
$$\times\,\mathcal{H}_0[\tau(\vec{R}_n)\,\psi(\vec{r};\,n\vec{\kappa}\sigma)]\ , \tag{B1}$$

where we have used the fact that the MTO are unitary. The requirement that the functions $\psi(\vec{r},\,n\vec{\kappa}\sigma)$ form a basis for the irreducible representations of $\tau(\vec{R}_n)$ [Eq. (2.3)] leads to

$$\langle n'\vec{\kappa}'\sigma'|\mathcal{H}_0|n\vec{\kappa}\sigma\rangle=\sum_{\sigma''\sigma'''}\Gamma^{\vec{\kappa}'}_{\sigma''',\sigma'}{}^*(\vec{R}_n)\ \Gamma^{\vec{\kappa}}_{\sigma'',\sigma}$$
$$\times\ (\vec{R}_n)\langle n'\vec{\kappa}'\sigma'''|\mathcal{H}_0|n\vec{\kappa}\sigma''\rangle\ . \tag{B2}$$

Summing both sides of Eq. (B2) over all values of $\vec{R}_n$ and using Eq. (A8), we obtain

$$\langle n'\vec{\kappa}'\sigma'|\mathcal{H}_0|\,n\vec{\kappa}\sigma\rangle=\delta_{\vec{\kappa}',\vec{\kappa}}\,\delta_{\sigma',\sigma}$$
$$\times\frac{1}{N}\sum_{\sigma''}\langle n'\vec{\kappa}\sigma''|\mathcal{H}_0|n\vec{\kappa}\sigma''\rangle \tag{B3}$$

Thus, the matrix element is dependent on σ.

APPENDIX C

In this Appendix we outline a formal prescription for finding the eigenvalues of $\mathcal{H}_0$. We assume the periodic potential possesses orthorhombic symmetry. One of the primitive lattice vectors is in the direction of magnetic field $\vec{a}_3\parallel\hat{z}_0\parallel\vec{b}$. We write

$$\psi(\vec{r})=\sum_{nj\lambda\vec{\kappa}\sigma}C_{nj\lambda}(\vec{\kappa},\,\sigma)\,\phi(\vec{r};\,nj\lambda,\,\vec{\kappa}\sigma)\ , \tag{C1}$$

where $\psi(\vec{r})$ is taken to be an eigenfunction of $\mathcal{H}_0$, and $\phi(r,\,nj\lambda,\,\vec{\kappa}\sigma)$ is an empty-lattice eigenfunction (see Appendix A). Inserting Eq. (B1) into Schrödinger's equation $\mathcal{H}_0\psi(\vec{r})=\epsilon\psi(\vec{r})$ leads to

$$\sum_{nj\lambda}\left\{\sum_{m_1,m_2}V_{m_1,m_2,j'-j}\,e^{i(m_1\kappa_ya_2-m_2\kappa_xa_1)N/s}\,e^{i2\pi m_1\lambda'/s}\,f_{n'n}(m_1,\,m_2)\,\delta_{\lambda'-\lambda,m_2N}\ (\text{modulo-}s)\right.$$

$$+\left[(n+\tfrac{1}{2})\frac{\hbar^2 b}{m}+\frac{\hbar^2}{2m}\left(\kappa_z+\frac{2\pi j}{a_3}\right)-\epsilon\right]\delta_{n'n}\,\delta_{j'j}\,\delta_{\lambda'\lambda}\Big\}C_{nj\lambda}(\vec{\kappa},\sigma)=0\ , \tag{C2}$$

where we have Fourier analyzed the periodic potential. In Eq. (C2)

$$V_{m_1,m_2,j'-j}=\Delta^{-1}\int_\Delta d^3x\,V(x,y,z)\exp\left[-i\left(\frac{2\pi m_1}{a_1}\,x+\frac{2\pi m_2}{a_2}\,y+\frac{2\pi(j'-j)}{a_3}\,z\right)\right] \tag{C3}$$

and

$$f_{n'n}(m_1,m_2)=\int_{-\infty}^{+\infty}d\xi\,\exp\left(\frac{i2\pi m_2\xi}{a_2b^{1/2}}\right)v_{n'}\left[b^{-1/2}\left(\xi+m_1\frac{N}{s}\,a_2b^{1/2}\right)\right]v_n(b^{-1/2}\xi)\ , \tag{C4}$$

where v_n is defined by equation (A3). $f_{n'n}(m_1, m_2)$ can be evaluated in closed form,

$$f_{n'n}(m_1,m_2)=\left(\frac{2^n}{2^{n'}}\right)^{1/2}\left(\frac{n!}{n'!}\right)^{1/2}e^{-i2\pi m_1m_2N/s}\left[m_1\left(\frac{a_2}{a_1}\right)^{1/2}+i\,m_2\left(\frac{a_1}{a_2}\right)^{1/2}\right]^{n'-n}\left(\frac{2\pi N}{s}\right)^{(n'-n)/2}$$

$$\times\exp\left[-\frac{\pi}{2}\,\frac{N}{s}\left(m_1^2\,\frac{a_2}{a_1}+m_2^2\,\frac{a_1}{a_2}\right)\right]L_n^{n'-n}\left[\frac{\pi N}{s}\left(m_1^2\,\frac{a_2}{a_1}+m_2^2\,\frac{a_1}{a_2}\right)\right], \tag{C5}$$

where $L_n^{n'-n}$ is an associated Laguerre polynominal.[18] In Eq. (C3) modulo s means that whenever m_2N is greater than s, the selection rule is $\delta_{\lambda'-\lambda,\,m_2N-\overline{m}s}$, where $\overline{m}$ is an integer chosen so that $m_2N-\overline{m}s$ is less than s.

Equation (C2) provides us with a secular equation for ϵ. The quantity in square brackets is independent of σ, and for a given value of $\vec{\kappa}$ and any σ, the secular equation yields an infinite number of eigenvalues. The eigenvalues, denoted by $\epsilon(n, \vec{\kappa})$ are, for a given $\vec{\kappa}$, numbered in order of increasing energy.

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*Work supported by the U. S. Air Force Office of Scientific Research under Grant No. AFAFOSR 62-258 and Contract No. AF 49(638)-1372.

†Work based on a dissertation submitted to the Polytechnic Institute of Brooklyn in partial fulfillment of the requirements for the degree of Doctor of Philosophy (unpublished).

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