Hall Effect in the Polaron-Band Regime*

L. FRIEDMAN
RCA Laboratories, Princeton, New Jersey
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A Hall effect is calculated for the band motion of the small polaron. The basic approach is to construct classical, Bloch-type wave packets from plane-wave combinations of localized polaron states. In this connection, it is shown that the effects of the "magnetic phase factors," which multiply the electronic overlap integrals in the basic Hamiltonian, are contained entirely in the conventional magnetic part, $(e/c)[\mathbf{v}_\sigma \times \mathbf{H}]$, of the total Lorentz force. The solutions of the steady-state Boltzmann equation for representative lattice structures indicate that the Hall coefficient is larger than or comparable to the "normal" value ($R=-1/nec$) according to whether or not three sites of the lattice are mutually nearest neighbors. Such a result was previously obtained in the alternate regime in which small polaron motion is due to hopping between local sites.

INTRODUCTION

IN a previous paper,[1] a nonvanishing Hall effect was theoretically predicted for the thermally activated hopping motion of the small polaron. Such a conduction mechanism, as has been discussed at length,[2] is prevalent at temperatures above a certain transition temperature T_t, which is $\sim\frac{1}{2}$ the Debye temperature, Θ. This result is of some interest, since it provides an example[3] of the existence of a Hall effect in hopping-type electronic transport.

However, as has been discussed in II, at sufficiently low temperatures ($T<T_t$) small polaron motion takes place in a band whose width J_p is an exponentially decreasing function of temperature.[2,4,5] The treatment of the Hall effect in this regime turns out to be formally similar to that of a conventional energy band. The only distinguishing feature with important physical consequences, as will be seen later, is the extreme smallness of the polaron bandwidth J_p with respect to $\kappa_B T$. However, for this and other reasons which appear immediately below, the calculation is of interest in its own right, and is the subject of the present paper.

In the polaron-band regime, the appropriate zeroth-order states are plane-wave combinations of localized polaron states (i.e., states describing the localized electron with its surrounding induced lattice deformation). The basic approach used in the calculation is to construct Bloch-type wave packets from these plane-wave states. It is shown that these wave packets propagate in $\boldsymbol{\sigma}$ space[6] according to a classical Lorentz force equation. In this connection, it is of particular interest that the effects of the "magnetic phase factors,"[7-9] $\alpha_{\mathbf{g},\mathbf{g}+\mathbf{h}}$, which were crucial in giving rise to a Hall effect in the site-jump regime, are shown to be contained *entirely* in the conventional magnetic component $(e/c)[\mathbf{v}_\sigma \times \mathbf{H}]$ of the total Lorentz force. Such a result is expected in the classical correspondence limit. More generally, the derivation of this result applies to any standard *tight-binding* treatment of band motion in which the effects of the applied magnetic field are formulated in terms of the above factors. To emphasize this point, in Appendix A, we sketch the derivation for the conventional atomic tight-binding case discussed by Zil'berman.[9]

The Lorentz force term derived by this procedure then plays the role of the driving term in a Boltzmann equation describing the polaron-band motion. A relaxation time assumption is made for the scattering term, with the relaxation time taken to be a constant.[10]

The Boltzmann equation is then solved to lowest order in H by the iteration method of Jones and Zener.[11] It is solved for three representative two-dimensional lattice structures, namely, square, face-centered, and (equilateral) triangular arrays.

Next, the currents (to order H) are found from the distribution functions in the standard way. In this connection, the integrations over the reduced wave-vector zone are facilitated by an important and distinguishing feature of the present calculation, namely, the previously mentioned smallness of the polaron bandwidth J_p with respect to $\kappa_B T$, i.e., $J_p \ll \kappa_B T$. As a consequence of this inequality, the currents are calculated to the lowest nonvanishing order[12] in $(J_p/\kappa_B T)$. From the symmetry of the band structure, it turns out that one must go to one higher order in this parameter for the square and face-centered lattices than for the three-site

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[1] L. Friedman and T. Holstein, Ann. Phys. (N. Y.) **21**, 494 (1963); hereafter to be referred to as III.

[2] T. Holstein, Ann. Phys. (N. Y.) **8**, 343 (1959); hereafter to be referred to as II.

[3] For another example, that of the impurity conduction regime of a semiconductor, see T. Holstein, Phys. Rev. **124**, 1329 (1961).

[4] J. Yamashita and T. Kurosawa, J. Phys. Chem. Solids **5**, 34 (1958).

[5] G. L. Sewell, Phil. Mag. **3**, 1361 (1959).

[6] Here $\boldsymbol{\sigma}$ denotes the wave vector of the polaron. This is to be distinguished from $\mathbf{k}$, which will represent the wave vector of the lattice vibrations.

[7] See (1.5) of the present text; also, (1.24) of III.

[8] R. E. Peierls, Z. Physik **80**, 780 (1933).

[9] G. Zil'berman, Zh. Eksperim. i Teor. Fiz. **29**, 762 (1955) [translation: Soviet Phys.—JETP **2**, 650 (1956)].

[10] This is justified in the text.

[11] A. H. Wilson, *The Theory of Metals* (Cambridge University Press, London, 1953), 2nd ed., p. 224.

[12] In essence, the exponential Boltzmann factor giving the equilibrium occupancy of the polaron-band states, is expanded in a Taylor series about $(J_p/\kappa_B T)=0$. One retains the lowest order term for which the integral is nonvanishing.

structure. As a result, the Hall coefficients turn out to be structure-dependent in just the same way as in the site-jump regime. In particular, it is found that the Hall coefficient corresponding to the three-site structure is larger than "normal" ($R_{\text{normal}}=-1/nec$) by a factor ($\kappa_B T/J_p$). On the other hand, the square and body-centered structure give just the normal result. The orders of magnitude of these results correspond to those obtained in the high-temperature ($T>T_t$) hopping regime discussed in III. As will be seen in the text, this contrasting behavior follows solely from the form of the Boltzmann equation discussed above and the nature of the polaron band. As such, it applies to any non-degenerate distribution of carriers whose motion obeys a Boltzmann equation of similar form, and whose energy band is of sufficiently narrow width (due to temperature-dependent vibrational narrowing or otherwise).

I. BASIC EQUATION OF MOTION AND APPROPRIATE ZEROTH-ORDER STATES

The present treatment is based on a suitable generalization of the one-dimensional molecular-crystal model (MCM) introduced in I and II. This model contains the basic features of the real physical situation, and serves as a convenient example of the small polaron mechanism. The above-mentioned generalization consists of extending the MCM to a two-dimensional crystal lattice and to the case of applied dc electric and magnetic fields. This has been described in detail in III. For the sake of completeness, however, we here discuss the essential features of the model, referring the reader to III for further details. Those features of the later calculation which are thought to be of a particularly general nature will be pointed out as they arise.

The crystal lattice is characterized by the vector site indexes

$$\mathbf{g}=g_1\mathbf{a}_1+g_2\mathbf{a}_2,$$

where $(\mathbf{a}_1,\mathbf{a}_2)$ are a basic set of lattice displacement vectors and (g_1,g_2) are integers. These lattice points are occupied by a set of N diatomic molecules with fixed centers of gravity and orientations (taken to be normal to the plane of the two-dimensional crystal, for reasons discussed in III), but with variable internuclear separations. Specifically, the "lattice Hamiltonian" in the absence of the excess electron, is assumed to have the form

$$H_L=\sum_{\mathbf{g}}\{(P_{\mathbf{g}}^2/2M)+\tfrac{1}{2}M\omega_0^2x_{\mathbf{g}}^2+\tfrac{1}{2}\sum_{\mathbf{h}}M\omega_1^2x_{\mathbf{g}}x_{\mathbf{g}+\mathbf{h}}\}. \quad (1.1)$$

Here, the $x_{\mathbf{g}}$ are the deviations from equilibrium of the internuclear separations of the individual molecules. The first two terms in (1.1) represent the kinetic and potential energies of the isolated molecules, while the third term provides nearest neighbor vibrational coupling (the sum over $\mathbf{h}$ goes over all nearest neighbors $\mathbf{g}+\mathbf{h}$, of site $\mathbf{g}$).

The motion of the excess electron (or hole) in this two-dimensional molecular crystal is formulated in terms of a tight-binding approximation, in which the state of the system is written as a linear superposition,

$$\Psi(\mathbf{r},\cdots x_{\mathbf{g}}\cdots)=\sum_{\mathbf{g}}a(\mathbf{g},\cdots x_{\mathbf{g}}\cdots)\phi_{\mathbf{g}}(\mathbf{r},x_{\mathbf{g}}), \quad (1.2)$$

of a basic set of "molecular" electronic wave functions, $\phi_{\mathbf{g}}(\mathbf{r},x_{\mathbf{g}})$. In the presence of a magnetic field, and with the assumptions[13] made in III, this set of basis functions turns out to be related to the set of local molecular wave functions $\phi(\mathbf{r}-\mathbf{g},x_{\mathbf{g}})$ (which apply for the case of zero magnetic field), *solely*[13] by the gauge transformation

$$\phi_{\mathbf{g}}(\mathbf{r},x_{\mathbf{g}})=\exp\{-ie[\mathbf{H}\times\mathbf{g}]\cdot\mathbf{r}/2\hbar c\}\phi(\mathbf{r}-\mathbf{g},x_{\mathbf{g}}). \quad (1.3)$$

The coefficients $a(\mathbf{g},\cdots x_{\mathbf{g}}\cdots)$ of the superposition (1.2) are each functions of all the $(\cdots x_{\mathbf{g}}\cdots)$. The equations which they obey are obtained from the time-dependent Schrödinger equation of the system by the standard "projection" procedure. With approximation appropriate to the tight-binding case, the large mass ratio of electrons and nuclei, as well as three additional simplifications of the model (see III, footnote 2), they take the form

$$i\hbar\frac{\partial a(\mathbf{g},\cdots x_{\mathbf{g}}\cdots)}{\partial t}$$
$$=[H_L+E(x_{\mathbf{g}})+e\mathbf{F}\cdot\mathbf{g}]a(\mathbf{g},\cdots x_{\mathbf{g}}\cdots)$$
$$-J\sum_{\mathbf{h}}\exp(i\alpha_{\mathbf{g},\mathbf{g}+\mathbf{h}})a(\mathbf{g}+\mathbf{h},\cdots x_{\mathbf{g}}\cdots). \quad (1.4)$$

Here, the "magnetic" phase factors $\alpha_{\mathbf{g},\mathbf{g}+\mathbf{h}}$ arise essentially from the gauge factors appearing in (1.3), and are given by[14]

$$\alpha_{\mathbf{g},\mathbf{g}+\mathbf{h}}=-(e/2\hbar c)\mathbf{H}\cdot[(\mathbf{g}+\mathbf{h})\times\mathbf{g}]. \quad (1.5)$$

The quantity $E(x_{\mathbf{g}})$ is the energy eigenvalue of the system consisting of the excess electron (or hole) and the gth isolated molecule. As discussed in III, the $x_{\mathbf{g}}$ dependence of $E(x_{\mathbf{g}})$, which essentially represents the electron-lattice interaction, is taken to be linear:

$$E(x_{\mathbf{g}})=-Ax_{\mathbf{g}}. \quad (1.6)$$

Finally, the term $e\mathbf{F}\cdot\mathbf{g}$ gives the electric field induced energy at site $\mathbf{g}$ ($\mathbf{F}$ being the electric field vector), and $-J$ is the standard electronic-overlap integral of tight-binding theory,

$$-J=\int dV\,\phi(\mathbf{r}-\mathbf{g})U(\mathbf{r}-\mathbf{g})\phi(\mathbf{r}-\mathbf{g}-\mathbf{h}), \quad (1.7)$$

[13] For purposes of treating the Hall effect, the effects of the magnetic field are considered only to terms linear in $\mathbf{H}$. In addition, it is assumed (a) that both $\mathbf{H}$ and the vibration axes of the diatomic molecules are perpendicular to the plane of the crystal, and (b) that the local functions $\phi(\mathbf{r}-\mathbf{g},x_{\mathbf{g}})$ are Σ states ($l_z=0$). These assumptions have the simplifying feature of introducing no magnetic-field dependence (to first order) into the wave functions pertaining to the isolated molecules. The phase factors appearing in (1.3) are entirely a consequence of the "projection" procedure of tight-binding theory (see III).

[14] This particular form of the phase factors arises from the use of the "symmetrical" gauge, $\mathbf{A}=\frac{1}{2}[\mathbf{H}\times\mathbf{r}]$. The question of gauge invariance is discussed in III, Appendix E.

taken to be a constant for all pairs of nearest neighbor sites $\mathbf{g}$, $(\mathbf{g}+\mathbf{h})$. Here, $U(\mathbf{r}-\mathbf{g})$ is the contribution of the molecule to the effective one-electron potential, and we have set $x_{\mathbf{g}}=x_{\mathbf{g}+\mathbf{h}}=0$ in accordance with simplifications introduced in III.

Transforming from the internuclear-displacement coordinates $(\cdots x_{\mathbf{g}}\cdots)$ to the normal-mode coordinates of the host crystal $(\cdots q_k\cdots)$ by means of the transformation

$$x_{\mathbf{g}}=(2/N)^{1/2}\sum_{\mathbf{k}} q_k \sin(\mathbf{k}\cdot\mathbf{g}+(\pi/4)),$$

and introducing (1.6), Eqs. (1.4) take the form

$$\begin{aligned} i\hbar\frac{\partial a(\mathbf{g},\cdots q_k\cdots)}{\partial t} &= \sum_{\mathbf{k}}\left\{-\frac{\hbar^2}{2M}\frac{\partial^2}{\partial q_k{}^2}+\frac{M\omega_k{}^2}{2}q_k{}^2-\left(\frac{2}{N}\right)^{1/2}Aq_k\right. \\ &\left.\times\sin(\mathbf{k}\cdot\mathbf{g}+(\pi/4))+e\mathbf{F}\cdot\mathbf{g}\right\}a(\mathbf{g},\cdots q_k\cdots) \\ &-J\sum_{\mathbf{h}}\exp(i\alpha_{\mathbf{g},\mathbf{g}+\mathbf{h}})a(\mathbf{g}+\mathbf{h},\cdots q_k\cdots), \end{aligned} \tag{1.8}$$

where

$$\omega_k{}^2=\omega_0{}^2+\omega_1{}^2\sum_{\mathbf{h}}\cos(\mathbf{k}\cdot\mathbf{h})$$

gives the dispersion of the vibrational spectrum. (Here and in what follows, we neglect the vector character of $\mathbf{k}$ when it appears as a subscript.)

Equation (1.8) is the basic starting point of the subsequent wave-packet analysis. Before going on to this, however, we first review zeroth-order eigenstates and eigenvalues appropriate to the local-site and polaron-band descriptions of the small polaron in the absence of applied fields ($\mathbf{F}=\mathbf{H}=0$).

As in II and III, the present treatment is restricted to the case for which the J-proportional term of (1.8) can be treated as a small perturbation. The conditions on J which insure the validity of this approximation are discussed in II, and are assumed to apply to the present case. The zeroth-order ($J=0$) eigenstates of (1.8) are

$$a_{\mathbf{g}_1}(\mathbf{g},\cdots q_k\cdots)=\delta_{\mathbf{g},\mathbf{g}_1}\chi_{\mathbf{g}_1\cdots N_k{}^{(1)}\cdots}(\cdots q_k\cdots), \tag{1.9}$$

where

$$\chi_{\mathbf{g}_1,\cdots N_k{}^{(1)}\cdots}(\cdots q_k\cdots)=\prod_{\mathbf{k}}\Phi_{N_k{}^{(1)}}[(M\omega_k/\hbar)(q_k-q_k{}^{(1)})] \tag{1.10}$$

represents a state of independent, displaced oscillators, $\Phi_{N_k}(z)$ being a normalized harmonic oscillator eigenfunction of excitation quantum number N_k, and

$$q_k{}^{(1)}=(2/N)^{1/2}(A/M\omega_k{}^2)\sin(\mathbf{k}\ \mathbf{g}_1+\tfrac{1}{4}\pi) \tag{1.11}$$

being the equilibrium normal-mode coordinates[15] corresponding to the electron being localized on site $\mathbf{g}_1$.

The eigenvalues corresponding to (1.9) are

$$E^{(0)}\cdots_{N_k{}^{(1)}}\cdots=E_b+\sum_{\mathbf{k}}\hbar\omega_k(N_k{}^{(1)}+\tfrac{1}{2}), \tag{1.12}$$

where

$$E_b=-\left(\frac{2}{N}\right)\sum_{\mathbf{k}}\frac{A^2}{2M\omega_k{}^2}\sin^2(\mathbf{k}\cdot\mathbf{g}+\tfrac{1}{4}\pi) \tag{1.13}$$

is the polaron binding energy.[15]

Physically, these zeroth-order eigenstates and eigenvalues correspond to the situation in which the electron is localized at site $\mathbf{g}_1$, and the vibrational state of the system specified by the set of quantum numbers $(\cdots N_k{}^{(1)}\cdots)$, giving the degree of excitation of each vibrational mode. It is to be noted that these modes differ from the purely lattice vibrational modes (which apply in the absence of the electron) only to the extent that the equilibrium values of the normal-mode coordinates depend on the site occupied by the electron.

For nonvanishing (but small) J, the time development of the system is treated by standard time-dependent perturbation theory. Specifically, the "wave function" of the system, $a(\mathbf{g},\cdots q_k\cdots)$, is expanded in the zeroth order, "local-site" representation (1.9). The coefficients in this expansion are found to develop according to certain characteristic matrix elements of the perturbation [i.e., of the J-proportional term of (1.8)] which are of the form

$$\begin{aligned} &(\mathbf{g}_2,\cdots N_k{}^{(2)}\cdots|V|\mathbf{g}_1,\cdots N_k{}^{(1)}\cdots) \\ &=-J\prod_{\mathbf{k}}\int\cdots\int\cdots\left(\frac{M\omega_k}{\hbar}\right)dq_k\cdots \\ &\times\Phi_{N_k{}^{(2)}}\left[\left(\frac{M\omega_k}{\hbar}\right)^{1/2}(q_k-q_k{}^{(2)})\right] \\ &\times\Phi_{N_k{}^{(1)}}\left[\left(\frac{M\omega_k}{\hbar}\right)^{1/2}(q_k-q_k{}^{(1)})\right]. \end{aligned} \tag{1.14}$$

These matrix elements clearly give rise to site jump transitions $\mathbf{g}_1\rightarrow\mathbf{g}_2$. One distinguishes the so-called "diagonal" transitions in which *all* the N_k remain unchanged, from the "nondiagonal" transitions in which one or more N_k change by ±1. It turns out that the diagonal transitions *alone* characterize the polaron-band motion. It is shown in II, that by taking only these into account, the appropriate eigenstates are plane-wave combinations of (1.9), namely,

$$a_{\sigma,\cdots N_k\cdots}=\exp(i\mathbf{g}\cdot\sigma)\chi_{\mathbf{g},\cdots N_k\cdots}, \tag{1.15}$$

[15] This arises as a result of incorporating the linear electron-lattice interaction term $(-Ax_{\mathbf{g}})$ in zeroth order.

with corresponding eigenvalues

$$E_{\sigma,\cdots N_k\cdots}=E^{(0)}{}_{\cdots N_k\cdots}-Je^{-S(\cdots N_k\cdots)}\times\sum_{\mathbf{h}}\exp(i\boldsymbol{\sigma}\cdot\mathbf{h}),\quad(1.16)$$

[cf. (35) and (36) of II].

Here, the polaron-band states are labeled by a wave-vector $\boldsymbol{\sigma}$, whose components in two-dimensional reciprocal wave-vector space are given by

$$\sigma_i=(2\pi/N_ih_i)n_i,$$

where n_i is an integer whose range is

$$-(N_i-1)/2<n_i\leq\tfrac{1}{2}(N_i-1),$$

and N_i is the number of molecular sites in the direction i (assumed odd for definiteness; $N=N_1\cdot N_2$ gives the total number of molecules).

The "vibrational overlap" factor, $e^{-S(\cdots N_k\cdots)}$, is nothing more than the diagonal matrix element of (1.14) (aside from the electronic overlap factor $-J$), i.e.,

$$e^{-S(\cdots N_k{}^{(1)}\cdots)}=\prod_{\mathbf{k}}\int\cdots\int\cdots\left(\frac{M\omega_k}{\hbar}\right)dq_k\cdots\times\Phi_{N_k{}^{(1)}}\left[\left(\frac{M\omega_k}{\hbar}\right)^{1/2}(q_k-q_k{}^{(2)})\right]\times\Phi_{N_k{}^{(1)}}\left[\left(\frac{M\omega_k}{\hbar}\right)^{1/2}(q_k-q_k{}^{(1)})\right].\quad(1.17)$$

Here, the quantity S is given by

$$S(\cdots N_k\cdots)=\sum_{\mathbf{k}}(1+2N_k)\gamma_k/N,\quad(1.18)$$

where

$$\gamma_k=\frac{A^2}{2M\omega_k{}^2\hbar\omega_k}(1-\cos\mathbf{k}\cdot\mathbf{h})$$

are the characteristic coupling constants of the theory. Apart from the trigonometric factor, they give the ratio of the polaron binding energy [cf (1.13)] to the vibrational quantum, $\hbar\omega_k$.

Finally, it is to be pointed out that the polaron bandwidth $J_p\sim Je^{-S(\cdots N_k\cdots)}$ is, by virtue of (1.18), an exponentially decreasing function of the N_k, and, hence, of temperature.[2,4,5] Even at $T=0$, $S(\cdots O_k\cdots)$ may be expected to be of the order of 5–10, so that the factor e^{-S}, which gives the ratio of the polaron bandwidth to the original electronic bandwidth, will be quite small ($\sim10^{-2}$–10^{-4}). As a consequence, the inequality

$$J_p\ll\kappa_BT$$

is readily satisfied, a feature crucial to the treatment of Sec. IV.

II. CLASSICAL WAVEPAC-KET TREATMENT

As discussed in the Introduction, our basic approach is to construct classical, Bloch-type wave packets from plane-wave combinations of localized polaron states (1.15), and to show that these propagate in $\boldsymbol{\sigma}$ space according to a conventional Lorentz force law. This result is to be derived from our basic equation (1.8), wherein the effects of the applied magnetic field are given by the "magnetic" phase factors $\alpha_{\mathbf{g},\mathbf{g}+\mathbf{h}}$ defined by (1.5). It will be later noted that this behavior applies to any conventional tight-binding[16] treatment of band motion in which the effects of the magnetic field are likewise formulated. This is pointed out in more detail at the end of this section and in Appendix A, where an analogous wave-packet treatment is given for the more conventional and simpler atomic tight-binding case discussed by Zil'berman.[9]

Proceeding with the analysis, the packets are assumed to satisfy two basic conditions. The first is that

$$\Delta g\gg a,\quad(2.1)$$

where Δg is a linear dimension characterizing the size of the packet, and a is the lattice constant. As is well known, this condition implies that the extent of the packet in reciprocal wave-vector (σ) space is very much less than the reduced wave-vector zone ($\sim\pi/a$). The second condition is

$$G\gg\Delta g,\quad(2.2)$$

where G is the orbital radius of the packet in the applied magnetic field. This condition, which localizes the packet on its magnetic orbit, insures the validity of a classical description. It is readily satisfied in the present treatment of the Hall effect which is concerned only with arbitrarily small field strengths (in particular, with effects which are linear in H).

The wave-packet expansion of $a(\mathbf{g},\cdots q_k\cdots)$ [appearing in (1.8)] in terms of the states (1.15) is written in the form

$$a(\mathbf{g},\cdots q_k\cdots)=N^{-1/2}\sum_{\sigma',\cdots N_k'\cdots}c_{\sigma',\cdots N_k'\cdots}\exp[-i(E^{(0)}{}_{\cdots N_k'\cdots}/\hbar)t]\times\exp[i(\mathbf{g}-\mathbf{g}_0)\cdot\boldsymbol{\sigma}']\chi_{\mathbf{g},\cdots N_k'\cdots}(\cdots q_k\cdots).\quad(2.3)$$

The packet has arbitrary centroid $\mathbf{g}_0$. The expansion coefficients $c_{\sigma',\cdots N_k'\cdots}$ depend on all the vibrational quantum numbers as indicated. The use of the interaction picture eliminates the local energies $E^{(0)}{}_{\cdots N_k'\cdots}$ [cf. (1.12)] from the subsequent analysis.

Substituting (2.3) into (1.8), multiplying from the left

[16] It should be pointed that while the Lorentz force law follows for general packets of Bloch states, the particular methods of the present paper, in which H is essentially treated as a perturbation, apply only to the tight-binding case, for which the bandwidth $\ll$interband energies. For this case, H can be so treated, and one can confine oneself to a single band (i.e., to a single electron orbital).

by $N^{-1/2}\exp[-i(\mathbf{g}-\mathbf{g}_0)\cdot\boldsymbol{\sigma}]\chi_{\mathbf{g},\cdots N_k\cdots}$, summing over $\mathbf{g}$ and all the q_k, and making use of the orthogonality relations

$$\int_{-\infty}^{\infty}\cdots\int_{-\infty}^{\infty}\cdots\left(\frac{M\omega_k}{\hbar}\right)dq_k\cdots\chi_{\mathbf{g},\cdots N_k\cdots}\chi_{\mathbf{g},\cdots N_{k'}\cdots}\cdots = \delta_{\cdots N_k\cdots,\cdots N_{k'}\cdots}, \tag{2.4}$$

$$\sum_{\mathbf{g}}\exp[i(\boldsymbol{\sigma}-\boldsymbol{\sigma}')\cdot(\mathbf{g}-\mathbf{g}_0)]=N\delta_{\sigma\sigma'},$$

one gets

$$\begin{aligned}i\hbar\frac{\partial c_{\sigma,\cdots N_k\cdots}}{\partial t}&=N^{-1}\sum_{\mathbf{g},\sigma'}\exp[i(\mathbf{g}-\mathbf{g}_0)\cdot(\boldsymbol{\sigma}'-\boldsymbol{\sigma})]e(\mathbf{F}\cdot\mathbf{g})c_{\sigma',\cdots N_k\cdots}\\&+\sum_{\mathbf{g},\mathbf{h}}\exp(i\alpha_{\mathbf{g},\mathbf{g}+\mathbf{h}})\sum_{\sigma',\cdots N_{k'}\cdots}c_{\sigma',\cdots N_{k'}\cdots}N^{-1}\\&\times\exp[i(\mathbf{g}-\mathbf{g}_0)\cdot(\boldsymbol{\sigma}'-\boldsymbol{\sigma})]\exp(i\mathbf{h}\cdot\boldsymbol{\sigma}')\\&\times(\mathbf{g},\cdots N_k\cdots|V|\mathbf{g}+\mathbf{h},\cdots N_{k'}\cdots),\end{aligned}\tag{2.5}$$

where $(\mathbf{g},\cdots N_k\cdots|V|\mathbf{g}+\mathbf{h},\cdots N_{k'}\cdots)$ is given by (1.14).

As discussed at the end of Sec. I, for purposes of describing the polaron-band motion, only the "diagonal" elements ($N_{k'}=N_k$ for all k) of (1.14) are retained. Then, employing (1.17), (2.5) becomes

$$\begin{aligned}i\hbar\frac{\partial c_{\sigma,\cdots N_k\cdots}}{\partial t}&=N^{-1}\sum_{\mathbf{g},\sigma'}\exp[i(\mathbf{g}-\mathbf{g}_0)\cdot(\boldsymbol{\sigma}'-\boldsymbol{\sigma})]e(\mathbf{F}\cdot\mathbf{g})c_{\sigma',\cdots N_k\cdots}\\&-Je^{-S(\cdots N_k\cdots)}\sum_{\mathbf{g},\mathbf{h}}\exp(i\alpha_{\mathbf{g},\mathbf{g}+\mathbf{h}})N^{-1}\sum_{\sigma'}c_{\sigma',\cdots N_k\cdots}\\&\times\exp[i(\mathbf{g}-\mathbf{g}_0)\cdot(\boldsymbol{\sigma}'-\boldsymbol{\sigma})]\exp(i\mathbf{h}\cdot\boldsymbol{\sigma}'),\end{aligned}\tag{2.6}$$

where $S(\cdots N_k\cdots)$ is given by (1.18).

To simplify the subsequent notation, in what follows we set

$$c_{\sigma,\cdots N_k\cdots}=c_\sigma,$$
$$S(\cdots N_k\cdots)=S,$$

bearing in mind that c and S depend on the $(\cdots N_k\cdots)$.

The electric field-dependent term appearing on the right-hand side of (2.6) is handled in a manner analogous to Bethe and Sommerfeld's treatment[17] of the acceleration of Bloch wave packets in a constant electric field. Writing $\mathbf{g}=\mathbf{g}_0+(\mathbf{g}-\mathbf{g}_0)$, and representing the latter term by the operator $-i\,\mathrm{grad}_{\sigma'}$ in the usual way, one obtains

$$-iN^{-1}\sum_{\mathbf{g},\sigma'}c_{\sigma'}e\mathbf{F}\cdot\mathrm{grad}_{\sigma'}\times\exp[i(\boldsymbol{\sigma}'-\boldsymbol{\sigma})\cdot(\mathbf{g}-\mathbf{g}_0)]+e(\mathbf{F}\cdot\mathbf{g}_0)c_\sigma,$$

where use has been made of the first relation of (2.4) to simply the second term, which clearly represents the electric-field energy corresponding to the packet centroid. In treating the first term, one employs the standard procedure of replacing the dense sum over $\boldsymbol{\sigma}'$ by an integral, and integrating by parts. The integrated term vanishes, since c_σ is assumed to be finite only over a very narrow extension of reduced wave-vector space, in accordance with inequality (2.1). Again using (2.4), one gets

$$ie\mathbf{F}\cdot\mathrm{grad}_\sigma c_\sigma+e(\mathbf{F}\cdot\mathbf{g}_0)c_\sigma.\tag{2.7}$$

The corresponding treatment of the magnetic field-dependent term[16] [the second term on the right-hand side of (2.6)] is somewhat more complicated, but straightforward. Again writing $\mathbf{g}=\mathbf{g}_0+(\mathbf{g}-\mathbf{g}_0)$, and applying the cyclic property of the scalar triplet product to the definition (1.5), one has

$$\begin{aligned}\alpha_{\mathbf{g},\mathbf{g}+\mathbf{h}}&=-(e/2\hbar c)\mathbf{H}\cdot[\mathbf{h}\times\mathbf{g}_0]-(e/2\hbar c)\mathbf{H}\cdot[\mathbf{h}\times(\mathbf{g}-\mathbf{g}_0)]\\&=(e/2\hbar c)[\mathbf{H}\times\mathbf{g}_0]\cdot\mathbf{h}-(e/2\hbar c)[\mathbf{H}\times\mathbf{h}]\cdot(\mathbf{g}-\mathbf{g}_0).\end{aligned}$$

For the sum over $\mathbf{g}$, one gets

$$N^{-1}\sum_{\mathbf{g}}\exp\{i[(\boldsymbol{\sigma}'-\boldsymbol{\sigma})-(e/2\hbar c)(\mathbf{H}\times\mathbf{h})]\cdot(\mathbf{g}-\mathbf{g}_0)\}=\delta_{\sigma',\sigma+(e/2\hbar c)[\mathbf{H}\times\mathbf{h}]},$$

reducing this term to

$$\begin{aligned}&-Je^{-S}\sum_{\mathbf{h},\sigma'}c_{\sigma'}\exp\{i(\boldsymbol{\sigma}'+(e/2\hbar c)[\mathbf{H}\times\mathbf{g}_0])\cdot\mathbf{h}\}\times\delta_{\sigma',\sigma+(e/2\hbar c)[\mathbf{H}\times\mathbf{h}]}\\&=-Je^{-S}\sum_{\mathbf{h}}c_{\sigma+(e/2\hbar c)[\mathbf{H}\times\mathbf{h}]}\times\exp\{i(\boldsymbol{\sigma}+(e/2\hbar c)[\mathbf{H}\times\mathbf{g}_0])\cdot\mathbf{h}\}.\end{aligned}\tag{2.8}$$

It is convenient to define a kinetic wave vector $\boldsymbol{\kappa}$ corresponding to the packet centroid:

$$\boldsymbol{\kappa}\equiv\boldsymbol{\sigma}+\frac{e}{\hbar c}\mathbf{A}(\mathbf{g}_0)=\boldsymbol{\sigma}+\frac{e}{2\hbar c}[\mathbf{H}\times\mathbf{g}_0].\tag{2.9}$$

In addition, it is useful to define a new function of the kinetic momentum b_κ such that

$$b_\kappa\equiv c^{\kappa-(e/2\hbar c)[\mathbf{H}\times\mathbf{g}_0]}=c_\sigma.\tag{2.10}$$

Incorporating (2.7), (2.8), (2.9), and (2.10) into (2.6), one obtains

$$i\hbar\left(\frac{\partial b_\kappa}{\partial t}\right)_\sigma=e(\mathbf{F}\cdot\mathbf{g}_0)b_\kappa+ie\mathbf{F}\cdot\mathrm{grad}_\kappa b_\kappa-Je^{-S}\sum_{\mathbf{h}}b_{\kappa+(e/2\hbar c)[\mathbf{H}\times\mathbf{h}]}\exp(i\boldsymbol{\kappa}\cdot\mathbf{h}),\tag{2.11}$$

[17] H. Bethe and A. Sommerfeld, in *Handbuch der Physik*, edited by H. Geiger and Karl Scheel (Julius Springer-Verlag, Berlin, 1934), Vol. 24, p. 2. The difference is that the electron coordinate $\mathbf{r}$ here gets replaced by a discrete-site coordinate, $\mathbf{g}$.

where the subscript $\boldsymbol{\sigma}$ affixed to the time derivative denotes that $\boldsymbol{\sigma}$ is to be held fixed, in accordance with the original meaning of the term. In fact, since $\boldsymbol{\kappa}$ is time-dependent via the packet centroid, one has that

$$\left(\frac{\partial}{\partial t}\right)_{\sigma}=\left(\frac{\partial}{\partial t}\right)_{\kappa}+\left(\frac{d\boldsymbol{\kappa}}{dt}\right)\cdot\operatorname{grad}_{\kappa}.$$

From (2.9), noting that $\partial\mathbf{g}_0/\partial t=\langle\mathbf{v}_\kappa\rangle$ is the velocity of the packet centroid, one then has

$$\left(i\hbar\frac{\partial}{\partial t}\right)_{\sigma}=\left(i\hbar\frac{\partial}{\partial t}\right)_{\kappa}+i\frac{e}{2c}[\langle\mathbf{v}_\kappa\rangle\times\mathbf{H}]\cdot\operatorname{grad}_{\kappa}. \quad (2.12)$$

Similarly, the form of the electric field term of (2.11) follows from the fact that, with t held constant, derivatives with respect to $\boldsymbol{\sigma}$ can be replaced by corresponding derivatives with respect to $\boldsymbol{\kappa}$.

Further progress in the development of (2.11) is afforded by the fact that, since $\mathbf{h}$ is a relative site vector and H is arbitrarily small, $b_{\kappa+(e/2\hbar c)[\mathrm{H}\times\mathbf{h}]}$ may be expanded to first order.[18] Thus,

$$b_{\kappa+(e/2\hbar c)[\mathrm{H}\times\mathbf{h}]}\cong b_\kappa+\frac{e}{2\hbar c}[\mathbf{H}\times\mathbf{h}]\cdot\operatorname{grad}_{\kappa}b_\kappa$$

$$=b_\kappa+\frac{e}{2\hbar c}[\operatorname{grad}_{\kappa}b_\kappa\times\mathbf{H}]\cdot\mathbf{h}.$$

Again using the relation

$$\mathbf{h}\exp(i\boldsymbol{\kappa}\cdot\mathbf{h})=-i\operatorname{grad}_{\kappa}\exp(i\boldsymbol{\kappa}\cdot\mathbf{h}),$$

the last term of (2.11) may be written

$$E_\kappa b_\kappa-i\left(\frac{e}{2c}\right)[\mathbf{v}_\kappa\times\mathbf{H}]\cdot\operatorname{grad}_{\kappa}b_\kappa, \quad (2.13)$$

where

$$E_\kappa=-Je^{-S}\sum_{\mathbf{h}}\exp(i\boldsymbol{\kappa}\cdot\mathbf{h}),$$

$$\mathbf{v}_\kappa=\hbar^{-1}\operatorname{grad}_{\kappa}E_\kappa. \quad (2.14)$$

Since the packet is assumed to be finite over only a very narrow range of $\boldsymbol{\sigma}$ space, we may replace $\langle\mathbf{v}_\kappa\rangle$ by $\mathbf{v}_\kappa$ in the usual way. Using (2.12) and (2.13), (2.11) becomes

$$\left(\frac{\partial b_\kappa}{\partial t}\right)_{\kappa}=\frac{i}{\hbar}[e\mathbf{F}\cdot\mathbf{g}_0+E_\kappa]b_\kappa+\frac{e}{\hbar}\left\{\mathbf{F}+\frac{1}{c}[\mathbf{v}_\kappa\times\mathbf{H}]\right\}\cdot\operatorname{grad}_{\kappa}b_\kappa.$$

Now,

$$\frac{\partial}{\partial t}|b_\kappa|^2=\frac{\partial b_\kappa^*}{\partial t}b_\kappa+b_\kappa^*\frac{\partial b_\kappa}{\partial t},$$

where the asterisk denotes the complex-conjugate quantity. With

$$f_\kappa=|b_\kappa|^2,$$

and reinstating the $(\cdots N_k\cdots)$ which were suppressed just after (2.6), one obtains

$$\frac{\partial f_{\kappa,\cdots N_k\cdots}}{\partial t}=\frac{e}{\hbar}\left\{\mathbf{F}+\frac{1}{c}[v_{\kappa,\cdots N_k\cdots}\times\mathbf{H}]\right\}\cdot\operatorname{grad}_{\kappa}f_{\kappa,\cdots N_k\cdots}. \quad (2.15)$$

Equation (2.15) describes the time development of the wave packets in $\boldsymbol{\kappa}$ space corresponding to a given distribution of the vibrational quantum numbers, $(\cdots N_k\cdots)$. The final step, then, is to take the thermal average of (2.15) over a Boltzmann distribution. The average of an arbitrary function Q is defined by

$$\langle Q(\cdots N_k\cdots)\rangle_{\mathrm{av}}=Z^{-1}\sum_{\cdots N_k\cdots}Q(\cdots N_k\cdots)\times\exp\{-\beta\sum_{\mathbf{k}}\hbar\omega_k(N_k+\tfrac{1}{2})\},$$

where

$$Z=\sum_{\cdots N_k\cdots}\exp\{-\beta\sum_{k}\hbar\omega_k(N_k+\tfrac{1}{2})\}$$

is the vibrational partition function, and

$$\beta=1/\kappa_B T,$$

κ_B being Boltzmann's constant, and T the absolute temperature. Physically, this averaging process corresponds to viewing the classical motion of the wave packet, described by (2.15), against the "average background" of the lattice motions. Recalling the definitions (2.14), one must consider the average

$$\langle e^{-S(\cdots N_k\cdots)}f_{\kappa,\cdots N_k\cdots}\rangle_{\mathrm{av}},$$

where $S(\cdots N_k\cdots)$ is given by (1.18). This is evaluated most easily by recognizing that $e^{-S(\cdots N_k\cdots)}$ can be replaced[19] by $e^{-S(\cdots\langle N_k\rangle\cdots)}$ with but small fluctuations of order $1/N$. With the definitions

$$J_p\equiv Je^{-S(\cdots\langle N_k\rangle\cdots)}\equiv Je^{-S_T},$$

$$S_T=\sum_k\frac{\gamma_k}{N}\coth\left(\frac{\beta\hbar\omega_k}{2}\right), \quad (2.16)$$

$$f_\kappa\equiv\langle f_{\kappa,\cdots N_k\cdots}\rangle,$$

Eq. (2.15) becomes

$$\frac{\partial f_\kappa}{\partial t}=\frac{e}{\hbar}\left\{\mathbf{F}+\frac{1}{c}[\mathbf{v}_\kappa\times\mathbf{H}]\right\}\cdot\operatorname{grad}_{\kappa}f_\kappa, \quad (2.17)$$

[18] The condition here is $|\mathbf{h}|\ll\alpha_0$, where $\alpha_0=(\hbar c/eH)^{1/2}$ is the characteristic magnetic length.

[19] That is, letting $Q(\cdots N_k\cdots)=e^{-S(\cdots N_k\cdots)}$, with S given by the sum (1.18), it can be verified by explicit calculation that

$$\langle(Q-\langle Q\rangle)^2\rangle=\langle Q^2\rangle-\langle Q\rangle^2\sim 1/N,$$

i.e., that fluctuations of Q about $\langle Q\rangle$ are negligible.

where f_κ is the standard distribution function, as applied to a spatially homogeneous situation.

This is the general result: the Lorentz force term of the Boltzmann transport equation. It is again pointed out the magnetic part of this term arises from the phase factors $\alpha_{\mathbf{g},\mathbf{g}+\mathbf{h}}$, which *alone* contain the magnetic-field dependence of our starting equation (1.8).

For our purposes, since we will be considering the motion of the packet only for short times,[20] the packet centroid, $\mathbf{g}_0$, will not depart appreciably from its initial value which, for convenience, we take to be $\mathbf{g}_0=0$. Then, according to (2.9), $\boldsymbol{\kappa}$ may be replaced by $\boldsymbol{\sigma}$ in (2.17), giving

$$\frac{\partial f_\sigma}{\partial t}=\frac{e}{\hbar}\left\{\mathbf{F}+\frac{1}{c}[\mathbf{v}_\sigma\times\mathbf{H}]\right\}\cdot\mathrm{grad}_\sigma f_\sigma. \tag{2.18}$$

To obtain the entire Boltzmann equation, we augment (2.18) by the collision term for which we make a relaxation time assumption. As shown in II (footnote 20), the relaxation time representing the effects of the nondiagonal transitions, is a constant,[21] independent of $\boldsymbol{\sigma}$. The final stationary Boltzmann equation is

$$\frac{\partial f_\sigma}{\partial t}=0=\frac{e}{\hbar}\left\{\mathbf{F}+\frac{1}{c}[\mathbf{v}_\sigma\times\mathbf{H}]\right\}\cdot\mathrm{grad}_\sigma f_\sigma-\frac{f_\sigma-f_\sigma^{(0)}}{\tau}, \tag{2.19}$$

where

$$f_\sigma^{(0)}=Ae^{-E_\sigma/\kappa_B T} \tag{2.20}$$

is the equilibrium distribution function of the nondegenerate polaron gas, and A is a normalization constant determined by the condition

$$\int f_\sigma^{(0)}d\boldsymbol{\sigma}=n, \tag{2.21}$$

where the integration is over a reduced zone, and n is the density of the polaron gas.

Before concluding this section, it is of some value to stop and take note of what has been done. The wave-packet expansion (2.3) superimposes plane-wave combinations of localized polaron states with a distribution of $(\cdots N_k\cdots)$. However, in going from (2.5) to (2.6), we retain only the "diagonal" matrix elements ($N_k'=N_k$, for all k) which entirely characterize the polaron band motion. From this point on, then, the vibrational quantum numbers play a more or less passive role, their only important effect, as discussed previously, being to reduce the polaron bandwidth (in comparison with the original electronic bandwidth) via the vibrational overlap factor $e^{-S(\cdots N_k\cdots)}$. In fact, the entire dynamical behavior follows for a given $(\cdots N_k\cdots)$ as is evidenced by (2.15); subsequent averaging over a Boltzmann distribution of the $(\cdots N_k\cdots)$ then gives the result (2.17). The point here is that by suppressing the $(\cdots N_k\cdots)$ and replacing the polaron bandwidth by some characteristic bandwidth, one finds that an equation of the type (2.6) is obeyed by the "envelope" function c_σ in a conventional tight-binding description of band motion in which the effects of the magnetic field are likewise formulated in terms of the "magnetic phase factors" introduced by Peierls[8] and Zil'berman.[9] A particularly simple example in the atomic tight-binding scheme presented by Zil'berman. An outline of his calculation together with a wave-packet treatment analogous to the one presented in the text, is given in Appendix A.

III. SOLUTION OF THE BOLTZMANN EQUATION

It is apparent that the calculation has been reduced to the solution of a conventional Boltzmann transport equation (2.19) for an energy band of tight-binding form, where the polaron bandwidth $J_p=Je^{-S_T}$ [cf. (2.16)] replaces the electronic overlap integral J.

Adopting a Cartesian coordinate system with coordinate axes denoted by (1,2,3), taking $\mathbf{H}$ in the 3 direction, $\mathbf{F}$ in the (1,2) plane, and setting

$$f_\sigma=f_\sigma^{(0)}+g_\sigma,$$

(2.19) becomes

$$e[F_1v_1+F_2v_2]+\frac{eH}{\hbar c}\left[v_2\frac{\partial g_\sigma}{\partial\sigma_1}-v_1\frac{\partial g_\sigma}{\partial\sigma_2}\right]-\frac{g_\sigma}{\tau}=0, \tag{3.1}$$

where, as usual, only terms of first order in F are retained, and $f_\sigma^{(0)}$ makes no contribution to the magnetic term. Setting

$$g_\sigma=-\frac{\partial f_\sigma^{(0)}}{\partial E_\sigma}\phi_\sigma,$$

and replacing $\mathbf{v}_\sigma$ by $(1/\hbar)\,\mathrm{grad}_\sigma E_\sigma$, (3.1) becomes

$$\frac{eH}{\hbar^2c}\left(\frac{\partial E_\sigma}{\partial\sigma_2}\frac{\partial}{\partial\sigma_1}-\frac{\partial E_\sigma}{\partial\sigma_1}\frac{\partial}{\partial\sigma_2}\right)\phi_\sigma-\frac{\phi_\sigma}{\tau}=-\frac{e}{\hbar}\left[F_1\frac{\partial E_\sigma}{\partial\sigma_1}+F_2\frac{\partial E_\sigma}{\partial\sigma_2}\right]. \tag{3.2}$$

Since, for purposes of calculating the Hall effect, ϕ_σ is needed only to first order in H, (3.2) is solved by an iteration procedure.[22] To the desired order of accuracy, the solution[23] is

$$\phi_\sigma=\phi_\sigma^{(0)}+\phi_\sigma^{(1)}, \tag{3.3}$$

[20] That is, $\omega_c\tau\ll1$, where $\omega_c=\langle v_\sigma\rangle/G$ is the cyclotron frequency. If τ is due only to the nondiagonal transitions, which play the role of scattering between polaron-band states (see II), it is assumed that T is a substantial fraction of T_t, say $\sim\frac{1}{2}T_t$, so that, for sufficiently small H, this inequality is satisfied. Of course, for $T>T_t$, by definition, the band approximation and Boltzmann equation are no longer valid.

[21] As far as other scattering mechanisms are concerned, since the features of interest derive from effects other than the possible σ dependence of τ_σ, the latter will be taken to be a constant as a suitable first approximation.

[22] This is the method of Jones and Zener; see Ref. 11.

[23] This agrees with the expanded form of Wilson's Eq. (8.551.3).

where

$$\phi_\sigma^{(0)}=-\frac{e\tau}{\hbar}\left(F_1\frac{\partial E_\sigma}{\partial\sigma_1}+F_2\frac{\partial E_\sigma}{\partial\sigma_2}\right), \tag{3.4}$$

$$\phi_\sigma^{(1)}=\frac{e^2\tau^2H}{\hbar c}\left(\frac{\partial E_\sigma}{\partial\sigma_1}\frac{\partial}{\partial\sigma_2}-\frac{\partial E_\sigma}{\partial\sigma_2}\frac{\partial}{\partial\sigma_1}\right)\times\left(F_1\frac{\partial E_\sigma}{\partial\sigma_1}+F_2\frac{\partial E_\sigma}{\partial\sigma_2}\right). \tag{3.5}$$

The current is given by

$$\mathbf{j}=e\frac{2}{(2\pi)^2}\int\int\mathbf{v}_\sigma\phi_\sigma\frac{\partial f_\sigma^{(0)}}{\partial E_\sigma}d\sigma_1d\sigma_2, \tag{3.6}$$

from which the elements of the conductivity tensor σ_{ij} are defined by the relations

$$j_i=\sigma_{ij}F_j. \quad (i,j=1,2). \tag{3.7}$$

From the experimental condition that $j_2=0$, the Hall coefficient may be simply expressed in terms of the σ_{ij}. Neglecting correction of order H^2, we have that

$$R=(1/H)\sigma_{12}/\sigma_{11}^2. \tag{3.8}$$

In the next section, the σ_{ij} will be calculated for the energy band structures corresponding to the lattice geometries previously described. From (3.8), we then readily obtain the respective Hall coefficients.

IV. EXPLICIT STRUCTURE CALCULATIONS FOR THE HALL COEFFICIENTS

In this section, we solve for the elements σ_{ij} of the conductivity tensor for the two-dimensional square, face-centered, and triangular lattice structures. These will be described and discussed in turn.

Before getting into the calculations, it is convenient at this point to consider a feature common to all three cases, namely, the extreme smallness of the polaron bandwidth with respect to κ_BT. Specifically, in calculating the current (3.6), it suffices to expand the factor $(\partial f_\sigma^{(0)}/\partial E_\sigma)$ in a power series in E_σ/κ_BT to that order which gives the first nonvanishing contribution to j. Thus, with $f_\sigma^{(0)}=Ae^{-E_\sigma/\kappa_BT}$, one has that

$$\exp(-E_\sigma/\kappa_BT)=1-\frac{E_\sigma}{\kappa_BT}+\frac{1}{2}\left(\frac{E_\sigma}{\kappa_BT}\right)^2+\cdots,$$
$$\frac{\partial\exp(-E_\sigma/\kappa_BT)}{\partial E_\sigma}=-\frac{1}{\kappa_BT}+\frac{E_\sigma}{(\kappa_BT)^2}+\cdots. \tag{4.1}$$

This expansion will be used immediately below. We now turn to the various geometries.

Square Lattice

For this case, the relative-site vectors are given by

$$\mathbf{h}=a(\pm1,0), \text{ etc.},$$

where a is the lattice constant. From (2.14), recalling that $\boldsymbol{\kappa}$ is to be replaced by $\boldsymbol{\sigma}$, one has

$$E_\sigma=-2J_p(\cos\sigma_1a+\cos\sigma_2a), \tag{4.2}$$
$$(v_\sigma)_i=V\sin\sigma_ia, \quad (i=1,2),$$

where

$$V=2J_pa/\hbar \tag{4.3}$$

is a characteristic velocity, and

$$2J_p=2Je^{-S_T}$$

is the polaron bandwidth.

The integrations indicated in (3.6) are to be carried out over the reduced wave-vector zone, which, for this case, is given by

$$-\pi/a<\sigma_1, \quad \sigma_2\leq\pi/a.$$

The detailed calculations of the σ_{ij} and expressions for $\phi_\sigma^{(0)}$ and $\phi_\sigma^{(1)}$ are given in Appendix B. We will present only the final results. For the case of σ_{11}, the first nonvanishing contribution occurs for the first term in the expansion (4.1). Eliminating the normalization constant A of (2.20) by condition (2.21), one finds that

$$\sigma_{11}=\frac{ne^2\tau}{2\kappa_BT}V^2, \tag{4.4}$$

where V is given by (4.3).

As shown in Appendix B, one must go to the *second* term in expansion (4.1) to obtain a nonvanishing result for σ_{12}. The result is

$$\sigma_{12}=\frac{ne^3\tau}{4c}H\frac{V^4}{(\kappa_BT)^2}. \tag{4.5}$$

Substituting (4.4) and (4.5) into (3.8), one obtains

$$R_{SQ}=-1/nec, \tag{4.6}$$

the normal result.

Face-Centered Structure

The direct reciprocal lattice structures are shown in Fig. 1. We have

$$\mathbf{h}=a(\pm\tfrac{1}{2},\pm\tfrac{1}{2}), \tag{4.7}$$

and

$$E_\sigma=-4J_p\cos(\tfrac{1}{2}\sigma_1a)\cos(\tfrac{1}{2}\sigma_2a).$$

In Appendix B, we find that

$$\sigma_{11}=\frac{ne^2\tau}{4\kappa_BT}V^2,$$
$$\sigma_{12}=-\frac{ne^3\tau^2}{16c}\frac{V^4}{(\kappa_BT)^2}, \tag{4.8}$$

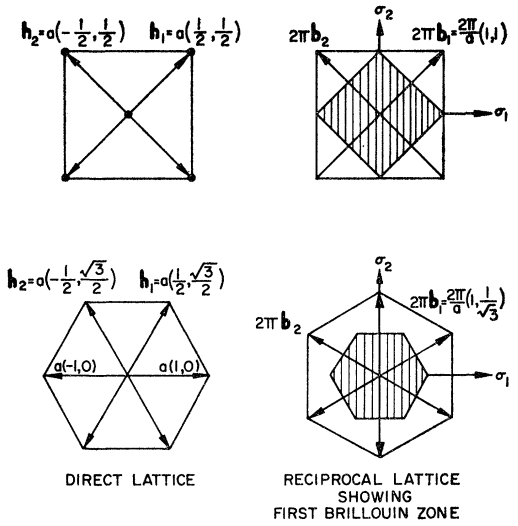

FIG. 1. Direct and reciprocal lattices for the face-centered and triangular structures.

where, again, one must go to the second term in the expansion (4.1) to obtain a nonvanishing contribution of σ_{12}. From (3.8) one finds that

$$R_{FC}=-1/nec, \tag{4.9}$$

again the normal result.

Triangular Lattice Structure

This structure has the property that the nearest neighbors of a given site are nearest neighbors of one another. Such an arrangement was crucial in giving a larger than normal Hall effect in the thermally activated hopping regime[24] discussed in paper III (Ref. 1). A similar order of magnitude result is obtained in the present case.

The direct and reciprocal lattices are shown in Fig. 1. The reduced zone is indicated by the shaded area. The band structure[25] is

$$E_\sigma=-2J_p[\cos\sigma_1 a+2\cos(\tfrac{1}{2}\sigma_1 a)\cos(\tfrac{1}{2}\sqrt{3}\sigma_2 a)]. \tag{4.10}$$

The detailed calculation for this case are presented in Appendix C. We find that

$$\sigma_{11}=-\frac{3}{4}\frac{ne^2\tau}{\kappa_B T}V^2. \tag{4.11}$$

However, in the calculation of σ_{12}, unlike the previous two cases, we obtain a nonvanishing contribution from the *first* term in the expansion (4.1). As a result, $\sigma_{12}\sim J^3$ rather than $\sim J^4$. We find

$$\sigma_{12}=-\frac{ne^2\tau^2}{(\hbar c)(\kappa_B T)}\frac{3}{16}aV^3, \tag{4.12}$$

and

$$R_3=-\frac{1}{nec}\frac{1}{6}\left(\frac{\kappa_B T}{J_p}\right), \tag{4.13}$$

which is the larger than normal result previously referred to.

It is to be noted that the results of this section follow solely from (2.19) and the inequality $J_p\ll\kappa_B T$. That is, once having established that the polaron packets propagate according to (2.19), and having assumed that their relaxation is characterized by a constant τ, the only specifically polaron-like feature upon which the above results depend is the vibrational narrowing of the polaron band. Hence, this behavior more generally applies to any narrow-band situation which satisfies the above conditions. The order of magnitude of the Hall coefficients for an energy- or wave-vector-dependent τ, or for those cases in which a relaxation time cannot be defined, would, however, require further investigation.

V. SUMMARY

The results of this paper are twofold. First, it has been shown that, in the classical limit, the effects of the "magnetic phase factors," $\alpha_{g,g+h}$, (which are quantum mechanical in origin) are given *entirely* by the conventional Lorentz force equation. Secondly, detailed calculations show that the Hall coefficient corresponding to a lattice geometry in which three sites are mutually nearest neighbors, is larger than "normal." The latter result was previously obtained in the high-temperature ($T>T_t$), thermally activated "hopping" regime of small polaron motion. There, this result was a reflection of the fact that the lowest order quantum mechanical interference process responsible for the Hall effect, is characteristic of the three-site geometry. In the present case of the polaron-band regime, however, the result arises as a consequence of the very narrow polaron bandwidths ($J_p\ll\kappa_B T$). These similarities suggest that the Hall effect in both regimes might eventually be treated and understood from a more unified point of view.

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APPENDIX A

In this Appendix, we redo the wave-packet analysis of Sec. II for the more conventional, and notationally

[24] The reason, essentially, is that the lowest order quantum mechanical interference process responsible for the Hall effect, is characteristic of such a geometry, and leads to a Hall current $\sim J^3$ (see III).

[25] Alternately, the calculation of the kinetic coefficients σ_{ij}, for this case, could be carried out in the coordinate system given by the basis vectors of the triangular lattice. In such a system, E_σ has a simple and symmetric form. However, this has the disadvantage that the diagonal and off-diagonal elements of σ_{ij} are no longer purely magnetic-field-independent and -dependent [to $O(H)$], respectively. Moreover, one must ultimately transform to Cartesian axes in order to evaluate R. Hence, it is simpler to work in such a system from the start, in spite of the unsymmetrical form of E_σ and its derivatives.

simpler atomic tight-binding case discussed by Zil'berman.[9] As has been pointed out in Ref. 3 (footnote 8), some modifications of his method are required to properly treat the present case.

Let $\phi_0(\mathbf{r})$ be the eigenfunction of the electron in an atom located at $\mathbf{n}=0$. Zil'berman derives the magnetic field H from the "unsymmetrical" gauge $\mathbf{A}=(0,Hx,0)$. For this case, the appropriate basis functions for an electron located at site $\mathbf{n}$, are, in analogy with (1.3) (also see Sec. 1 of III),

$$\phi_{\mathbf{n}}(\mathbf{r})=\exp\{-i\alpha_0^{-2}n_1(y-n_2)\}\phi_0(\mathbf{r}-\mathbf{n}), \quad \text{(A1)}$$

where $\alpha_0=(\hbar c/eH)^{1/2}$ is the characteristic "magnetic" length.

These functions satisfy the wave equations

$$\frac{1}{2m}\left\{p_1^2+\left[p_2+\frac{eHx}{c}\right]^2+p_3^2\right\}\phi_{\mathbf{n}} +[V(\mathbf{r}-\mathbf{n})+eF_2(y-n_2)]\phi_{\mathbf{n}}=E_{\mathbf{n}}\phi_{\mathbf{n}}, \quad \text{(A2)}$$

where $V(\mathbf{r}-\mathbf{n})$ is the atomic potential at site $\mathbf{n}$, and $F=F_2$ is the applied electric field. Substituting (A1) into (A2), one gets the equation obeyed by $\phi_0(\mathbf{r}-\mathbf{n})$:

$$\frac{1}{2m}\left\{p_1^2+\left[p_2+\frac{eH}{c}(x-n_1)\right]^2+p_3^2\right\}\phi_0 +[V(\mathbf{r}-\mathbf{n})+eF_2(y-n_2)]\phi_0=E_{\mathbf{n}}\phi_0. \quad \text{(A3)}$$

However, as a consequence of the gauge dependence of the Schrödinger equation, $\phi_0(\mathbf{r}-\mathbf{n})$ contains an implicit (linear) field dependence neglected by Zil'berman. To account for this, we introduce the additional gauge transformation

$$\phi_0(\mathbf{r}-\mathbf{n})=\exp[-\tfrac{1}{2}i\alpha_0^{-2}(x-n_1)(y-n_2)]\phi_{00}(\mathbf{r}-\mathbf{n}), \quad \text{(A4)}$$

from which it can be established that if, as implied by Zil'berman's treatment, the basis functions are nondegenerate atomic orbitals (and, therefore, an s states, $l_z=0$), ϕ_{00} is independent of magnetic field to order H^1. The entire magnetic-field dependence of the basic states is then given by the product of (A1) and (A4).

Getting back to the main trend of the argument, if we expand the wave function of the electron in the periodic field of the lattice in the representation of the $\phi_{\mathbf{n}}$,

$$\Psi=\sum_{\mathbf{n}} a_{\mathbf{n}}\phi_{\mathbf{n}}(\mathbf{r}) \quad \text{(A5)}$$

[cf. (1.2) of the present text], the expansion coefficients $a_{\mathbf{n}}$ are found to obey the equations of motion

$$\epsilon a_{\mathbf{m}}=\sum_{\mathbf{n}} a_{\mathbf{n}}\epsilon_{\mathbf{mn}} \quad \text{(A6)}$$

[cf. (1.4)].

Here $\epsilon=E-E_a$, E being the energy of the electron in the periodic potential, and E_a being the energy in the isolated atom. With the phase factors given by (A1) and (A4), the $\epsilon_{\mathbf{mn}}$ turn out to be

$$\epsilon_{\mathbf{mn}}=\exp\{\tfrac{1}{2}i\alpha_0^{-2}[(m_1-n_1)n_2-(m_2-n_2)n_1]\} \times[A(\mathbf{m}-\mathbf{n})+eF_2n_2\delta_{\mathbf{mn}}], \quad \text{(A7)}$$

where the exchange or overlap integral $A(\mathbf{q})$ is

$$A(\mathbf{q})=\int\phi_{00}(\mathbf{r}-\mathbf{q})[V_p(\mathbf{r})-V(\mathbf{r})]\phi_{00}(\mathbf{r})dV, \quad \text{(A8)}$$

V_p being the periodic potential and V the atomic potential.

We introduce the wave-packet expansion

$$a_{\mathbf{m}}=\sum_{\sigma} c_\sigma\exp[i\boldsymbol{\sigma}\cdot(\mathbf{m}-\mathbf{m}_0)] \quad \text{(A9)}$$

[cf. (2.3)] into (A5).

Considering the time-dependent analog of (A6) ($E\rightarrow i\hbar\partial/\partial t$), one gets the following equation of motion for the coefficients c_σ:

$$\left(i\hbar\frac{\partial}{\partial t}-E_a\right)c_\sigma =N^{-1}eF_2\sum_{\mathbf{m},\sigma'}\exp[i(\mathbf{m}-\mathbf{m}_0)\cdot(\boldsymbol{\sigma}'-\boldsymbol{\sigma})]c_{\sigma'} +\sum_{\mathbf{m},\mathbf{h}}\exp[i\alpha_0^{-2}(m_2h_1-m_1h_2)]A(\mathbf{h})\exp(-i\mathbf{h}\cdot\boldsymbol{\sigma}') \times\sum_{\sigma'}\exp[i(\mathbf{m}-\mathbf{m}_0)\cdot(\boldsymbol{\sigma}'-\boldsymbol{\sigma})]c_{\sigma'}, \quad \text{(A10)}$$

of the same form as text Eq. (2.5).

Treating the field-dependent terms of (A10) by arguments identical to those used in the text, one obtains

$$\frac{\partial f_\kappa}{\partial t}=\frac{eF_2}{\hbar}\frac{\partial f_\kappa}{\partial\kappa_2}+\frac{eH}{\hbar c}\left(v_2\frac{\partial f_\kappa}{\partial\kappa_1}-v_1\frac{\partial f_\kappa}{\partial\kappa_2}\right), \quad \text{(A11)}$$

where the components of the kinetic wave vector $\boldsymbol{\kappa}$ are

$$\kappa_1=\sigma_1-\tfrac{1}{2}\alpha_0^{-2}m_{02},$$
$$\kappa_2=\sigma_2+\tfrac{1}{2}\alpha_0^{-2}m_{01},$$
$$\kappa_3=\sigma_3.$$

Here, the distribution function f_κ is given by

$$f_\kappa=|b_\kappa|^2,$$

where

$$b_{\kappa_1,\kappa_2,\kappa_3}=c_{\kappa_1+\frac{1}{2}\alpha_0^{-2}m_{02},\kappa_2-\frac{1}{2}\alpha_0^{-2}m_{01},\kappa_3},$$

and the ith component of velocity of an electron in state $\boldsymbol{\kappa}$ is

$$v_i=\frac{1}{\hbar}\frac{\partial}{\partial\kappa_i}\sum_{\mathbf{h}}A(\mathbf{h})\exp(-i\boldsymbol{\kappa}\cdot\mathbf{h}).$$

This establishes the Lorentz force law for this case.

APPENDIX B

In this Appendix, we present the detailed expressions for $\phi_\sigma^{(0)}$, $\phi_\sigma^{(1)}$, and $\mathbf{j}$ for the case of the square and face-centered lattice structures.

Square Lattice

For the band structure (4.2), the expressions (3.4) and (3.5) become

$$\phi_\sigma^{(0)} = -e\tau V(F_1 \sin\sigma_1 a + F_2 \sin\sigma_2 a),$$
$$\phi_\sigma^{(1)} = \frac{e^2\tau^2 Ha}{\hbar c} V^2(F_1 \sin\sigma_1 a \cos\sigma_2 a - F_2 \cos\sigma_1 a \sin\sigma_2 a), \tag{B1}$$

where V is defined by (4.3).

We first calculate the current in the 1 direction associated with the magnetic-field-independent part of the distribution function $\phi_\sigma^{(0)}$. From (3.6), we have

$$j_1^{(0)} = \frac{2}{(2\pi)^2} eA \int_{-\pi/a}^{\pi/a}\int_{-\pi/a}^{\pi/a} d\sigma_1 d\sigma_2\, v_1 \phi_\sigma^{(0)} (\partial f_\sigma^{(0)}/\partial E_\sigma)$$
$$= \frac{1}{(2\pi)^2} e^2 V^2 \tau A \int_{-\pi/a}^{\pi/a}\int_{-\pi/a}^{\pi/a} d\sigma_1 d\sigma_2 \times \sin\sigma_1 a(F_1 \sin\sigma_1 a + F_2 \sin\sigma_2 a) \times \left\{ -\frac{1}{\kappa_B T} \exp\left[\frac{2J_p}{\kappa_B T}(\cos\sigma_1 a + \cos\sigma_2 a)\right]\right\}. \tag{B2}$$

It is obvious from symmetry considerations that the F_2-proportional term vanishes identically for arbitrary $(J_p/\kappa_B T)$. With regard to the F_1-proportional term, it clearly suffices to replace the Boltzmann exponential factor by unity [this corresponds to retaining only the first term in the expansion (4.1)].

Evaluating A by (2.21), we get

$$A = \tfrac{1}{2} n a^2.$$

This gives

$$\sigma_{11} = (ne^2\tau/2\kappa_B T) V^2, \tag{B3}$$

which is the text Eq. (4.4).

For the component of the current in the 1 direction associated the magnetic-field-dependent part $\phi_\sigma^{(1)}$, we have

$$j_1^{(1)} = \frac{2}{(2\pi)^2} \frac{e^3\tau^2 H}{\hbar c} V^3 A \int_{-\pi/a}^{\pi/a}\int_{-\pi/a}^{\pi/a} d\sigma_1 d\sigma_2 \sin\sigma_1 a \times (F_2 \sin\sigma_1 a \cos\sigma_2 a - F_1 \cos\sigma_1 a \sin\sigma_2 a) \times \left\{ -\frac{1}{\kappa_B T} \exp\left[\frac{2J_p}{\kappa_B T}(\cos\sigma_1 a + \cos\sigma_2 a)\right]\right\}. \tag{B4}$$

The F_1-proportional term now vanishes by symmetry for arbitrary $(J_p/\kappa_B T)$. If the exponent were replaced by unity, the F_2-proportional term would also vanish; hence, the first nonvanishing contribution comes from the second term in the expansion of the exponent, corresponding to the second term in the expansion (4.1). As a result, $\sigma_{12} \sim J^4$. Specifically,

$$\sigma_{12} = -\frac{ne^3\tau^2}{4c} H \frac{V^4}{(\kappa_B T)^2}, \tag{B5}$$

which is the text Eq. (4.5). Using (B3) and (B5), we obtain the result (4.6) for the Hall coefficient.

Face-Centered Structure

Using (4.7), (3.4) and (3.5) take the form

$$\phi_\sigma^{(0)} = -e\tau V[F_1 \sin(\tfrac{1}{2}\sigma_1 a) \cos(\tfrac{1}{2}\sigma_2 a) + F_2 \cos(\tfrac{1}{2}\sigma_1 a) \sin(\tfrac{1}{2}\sigma_2 a)],$$
$$\phi_\sigma^{(1)} = \frac{e^2\tau^2 Ha}{2\hbar c} V^2[-F_1 \sin(\tfrac{1}{2}\sigma_2 a) \cos(\tfrac{1}{2}\sigma_2 a) + F_2 \sin(\tfrac{1}{2}\sigma_1 a) \cos(\tfrac{1}{2}\sigma_1 a)]. \tag{B6}$$

In performing the required integration over $\boldsymbol{\sigma}$ space to obtain the currents, one must strictly integrate over the reduced wave-vector zone shown in Fig. 1. Although this band structure is quite simple, we propose to carry out the integrations by an alternate approximate method which simplifies the calculation considerably in the case of more complex structures. The method consists of taking advantage of the periodicity in extended $\boldsymbol{\sigma}$ space by integrating over a large square containing many reduced zones, and dividing by the number of zones. In so doing, one makes an error proportional to the perimeter to area ratio which can be made arbitrary small for a sufficiently large square. This procedure will be applied to the triangular lattice structure presented in Appendix C, and will serve to simplify the calculation for more complex structures which may be considered in the future.

In the present case, we integrate over a square $(4\pi G/a)$ on an edge, and divide by the number of zones, which is $(4\pi G/a)^2/[\tfrac{1}{2}(4\pi/a)^2] = 2G^2$. Thus,

$$j_1^{(0)} = \frac{2}{(2\pi)^2} e^2\tau^2 V^2 A \frac{1}{2G^2} \times \int\int_{-2\pi G/a}^{2\pi G/a} d\sigma_1 d\sigma_2 \sin(\tfrac{1}{2}\sigma_1 a) \cos(\tfrac{1}{2}\sigma_2 a) \times [F_1 \sin(\tfrac{1}{2}\sigma_1 a) \cos(\tfrac{1}{2}\sigma_2 a) + F_2 \cos(\tfrac{1}{2}\sigma_1 a) \sin(\tfrac{1}{2}\sigma_2 a)] \times \left[-\frac{1}{\kappa_B T} \exp\left(\frac{4J_p}{\kappa_B T} \cos(\tfrac{1}{2}\sigma_1 a) \cos(\tfrac{1}{2}\sigma_2 a)\right)\right]. \tag{B7}$$

The normalization constant is readily found to be

$$A=\tfrac{1}{4}na^2.$$

Proceeding just as in the case of the square lattice, we get

$$\sigma_{11}=\frac{ne^2\tau}{4\kappa_BT}V^2. \tag{B8}$$

The expression for $j_1^{(1)}$ is

$$j_1^{(1)}=\frac{2}{(2\pi)^2}\frac{e^3\tau^2Ha}{2\hbar c}V^3\frac{1}{2G^2}$$
$$\times\int\int_{-2\pi G/a}^{2\pi G/a}d\sigma_1d\sigma_2\sin(\tfrac{1}{2}\sigma_1a)\cos(\tfrac{1}{2}\sigma_2a)$$
$$\times[F_1\sin(\tfrac{1}{2}\sigma_2a)\cos(\tfrac{1}{2}\sigma_2a)+F_2\sin(\tfrac{1}{2}\sigma_1a)\cos(\tfrac{1}{2}\sigma_1a)]$$
$$\times\left[-\frac{1}{\kappa_BT}\exp\left(\frac{4J_p}{\kappa_BT}\cos(\tfrac{1}{2}\sigma_1a)\cos(\tfrac{1}{2}\sigma_2a)\right)\right],$$

from which one obtains

$$\sigma_{12}=-\frac{ne^3\tau^2}{16c}H\frac{V^4}{(\kappa_BT)^2}. \tag{B9}$$

The result (4.9) then follows immediately.

APPENDIX C

In this Appendix, we present the detailed calculations for the case of the three-site geometry. Using (4.10), (3.4) and (3.5) become[25]

$$\phi_\sigma^{(0)}=-e\tau V[F_1(\sin\sigma_1a+\sin(\tfrac{1}{2}\sigma_1a)\cos(\tfrac{1}{2}\sqrt{3}\sigma_2a))$$
$$+F_2(\sqrt{3}\cos(\tfrac{1}{2}\sigma_1a)\sin(\tfrac{1}{2}\sqrt{3}\sigma_2a))], \tag{C1}$$

$$\phi_\sigma^{(1)}=-\frac{e^2\tau^2H}{\hbar c}V^2\sqrt{3}a\Big\{[\tfrac{1}{2}(\sin\sigma_1a+\sin(\tfrac{1}{2}\sigma_1a)\cos(\tfrac{1}{2}\sqrt{3}\sigma_2a))$$
$$\times\sin(\tfrac{1}{2}\sigma_1a)\sin(\tfrac{1}{2}3\sigma_2a)+\cos(\tfrac{1}{2}\sigma_1a)\sin(\tfrac{1}{2}\sqrt{3}\sigma_2a)$$
$$\times(\cos\sigma_1a+\tfrac{1}{2}\cos(\tfrac{1}{2}\sigma_1a)\cos(\tfrac{1}{2}\sqrt{3}\sigma_2a))]F_1-\tfrac{1}{2}\sqrt{3}$$
$$\times[(\sin\sigma_1a+\sin(\tfrac{1}{2}\sigma_1a)\cos(\tfrac{1}{2}\sqrt{3}\sigma_2a))$$
$$\times\cos(\tfrac{1}{2}\sigma_1a)\cos(\tfrac{1}{2}\sqrt{3}\sigma_2a)$$
$$+\cos(\tfrac{1}{2}\sigma_1a)\sin(\tfrac{1}{2}\sigma_1a)\sin^2(\tfrac{1}{2}\sqrt{3}\sigma_2a)]F_2\Big\}. \tag{C2}$$

We also have that

$$v_1=V[\sin\sigma_1a+\sin(\tfrac{1}{2}\sigma_1a)\cos(\tfrac{1}{2}\sqrt{3}\sigma_2a)], \tag{C3}$$

$$v_2=\sqrt{3}V\cos(\tfrac{1}{2}\sigma_1a)\sin(\tfrac{1}{2}\sqrt{3}\sigma_2a). \tag{C4}$$

We use the same method of integration as in the previous case. Here, however, it is more convenient to integrate over a large rectangle, $(4\pi G/a)$ along σ_1, $(4\pi G/\sqrt{3}a)$ along σ_2. The number of zones in the rectangle is

$$\frac{4}{\sqrt{3}}\left(\frac{2\pi G}{a}\right)^2\Big/\frac{2}{\sqrt{3}}\left(\frac{2\pi}{a}\right)^2=2G^2.$$

We also find that

$$A=\tfrac{1}{4}\sqrt{3}na^2.$$

Using (B1) and (B3) in (3.6), one obtains

$$\sigma_{11}=\frac{3}{4}\frac{ne^2\tau}{\kappa_BT}V^2. \tag{C5}$$

In calculating σ_{12}, one must consider the product of (C2) and (C3) in (3.6). A careful examination of the integrand shows that a finite contribution comes from the product of the first term of v_1 with the second term of the bracket multiplying F_2. Moreover, this contribution does *not* require expansion of the exponent, [i.e., corresponding to taking the first term in the expansion (4.1)]. One obtains

$$\sigma_{12}=-\frac{3}{16}a\frac{ne^3\tau^2H}{(\hbar c)(\kappa_BT)}V^3, \tag{C6}$$

and, finally,

$$R_3=-\frac{1}{nec}\frac{1}{6}\left(\frac{\kappa_BT}{J_p}\right), \tag{C7}$$

which is the result given by (4.13).