Hall Coefficient of Hubbard's Model*

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With the aid of the Kadanoff-Baym transport equations, the high-field Hall coefficient is calculated for holes in narrow bands according to Hubbard's model. It is found that the inverse Hall coefficient is proportional to the fraction of momentum space occupied by the holes, which in Hubbard's model does not equal the number of holes per atom. Therefore, the holes would not be compensated by the conduction electrons, and it is concluded that Hubbard's model in its present form is inapplicable to even-valence transition metals such as palladium and platinum.

I. INTRODUCTION

RECENTLY, there has been considerable experimental evidence for anomalies in the spectral density for d electrons in the transition metals[1,2] Ni, Pd, Pt. In Ni, for example, the spectral density appears to be split into two parts: the high-energy part resembles the expected band structure density of states; below it is split off a single peak of strength nearly equal to that of the higher part.

Hubbard[3,4] has proposed a microscopic model which under certain conditions gives split bands as suggested by experiment. For $\sim 0.5d$ holes per atom, Hubbard's theory gives peaks of about equal weight,[5] in agreement with the nickel data, but it predicts approximately equal widths, instead of one "band-like" and one "resonance-like" peak. Clearly it would be desirable to find further predictions of Hubbard's model to compare with experiment.[6]

For Hubbard's model to predict split bands, the effective intra-atomic Coulomb repulsion energy (I) must be $\gtrsim$ the bandwidth.[4] Various estimates[3,7–10] for I in transition metals (including the effect of s screening) have varied between ~ 0 and 15 eV. Recent experimental evidence[11] suggests that $I \sim 7$ eV in Ni, although the interpretation of the experiments depends, at least superficially, on Anderson's local moment theory,[7] whose validity is uncertain.[12,13] There seems to be little doubt, however, that I is sufficiently large in the rare earths. It may well be that Hubbard's theory is applicable to the rare earths, even if it should prove inapplicable (or uninteresting) in the transition metals.

As emphasized by Phillips,[2] an interesting property of a "resonance" or "split-band" model is that the Fermi surface need not enclose the same volume of momentum space as predicted by normal Fermi-liquid theory.[14,15] Indeed, Hubbard's model predicts that the fraction of momentum space occupied by the d holes is larger than the number of d holes per atom. Herring[16] has suggested that this may lead to incorrect predictions of the galvanomagnetic properties. The point is this: experimental evidence[17] indicates that the d holes of platinum and palladium are compensated by the s electrons in high magnetic fields. Presumably, then, the d holes must contribute a field-independent term $-n_h ec$ to the inverse Hall coefficient (R^{-1}) to cancel an identical term from the s electrons (which presumably form a normal system). We are thus led to ask whether Hubbard's model predicts that the hole contribution to R^{-1} is proportional to the density of holes, or whether it is proportional to the volume of momentum space occupied by the d holes (or to something else). In this

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[5] When the number (n_h) of d holes per atom is less than unity, Hubbard's "zero configuration width approximation" predicts that the lower peak contains $0.9\ n_h$ of the spectral weight.
[6] Hubbard [Proc. Phys. Soc. (London) **84**, 455 (1964)] has used his model to calculate the exchange splitting in Ni. This provides only an inclusive test of the theory, however, since one obtains about the same exchange splitting as predicted by Slater [Phys. Rev. **49**, 537 (1936)] from an entirely different mechanism.
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paper we make a detailed calculation to answer the question.

To do this calculation, we use the Kadanoff-Baym transport equations.[18] When applied to the simpler form of Hubbard's model, these equations reduce to a single equation analogous to the ordinary Boltzmann equation. In a high magnetic field this equation may be trivially solved for the conductivity. We find that R^{-1} is proportional to the volume of momentum space occupied by the holes, rather than to their density. Next we extend the analysis to include the various lifetime effects considered in Hubbard's third paper.[4] We find that R^{-1} is not qualitatively affected by these refinements, provided that the bandwidth is narrow enough that the bands remain well split. Our results depend only on certain general properties of Hubbard's Green's function, and on none of the specific details. It is concluded that Hubbard's model is probably not applicable to the even-valence transition metals, such as platinum and palladium.

II. HUBBARD'S MODEL

In what follows we consider only the simpler theory for a nondegenerate band. For thermal equilibrium, Hubbard writes the Green's function in the form[19]

$$G(\mathbf{p},z)=[F(z)-(\epsilon_\mathbf{p}-\bar{\epsilon})]^{-1}, \tag{1}$$

where $\epsilon_\mathbf{p}$ is the band energy and $\bar{\epsilon}$ is the mean band energy. According to Hubbard, the quantity $(\epsilon_\mathbf{p}-\bar{\epsilon})$ is to be thought of as describing the propagation of electrons between atoms and $F(z)$ the resonant properties of the atoms themselves. In the simplest approximation[3]

$$\frac{1}{F(z)}=\frac{1-\frac{1}{2}n}{z-\bar{\epsilon}}+\frac{\frac{1}{2}n}{z-\bar{\epsilon}-I}, \tag{2}$$

which resonates at frequencies corresponding to the difference between atomic levels. (In this approximation, the atomic levels occur at energies 0, $\bar{\epsilon}$, and $2\bar{\epsilon}+I$ corresponding to 0, 1, or 2 valence electrons, respectively, on the atom.) Here n is the number of electrons per atom, and I is the intra-atomic Coulomb repulsion energy mentioned earlier. The split bands predicted by Hubbard occur because the interatomic kinetic energy $(\epsilon_p-\bar{\epsilon})$ is too small (by assumption) to outweigh the atomic level splittings.

It is convenient to write the Green's function in the form

$$G(\mathbf{p},z)=[z-\epsilon_\mathbf{p}-\Sigma(z)]^{-1}, \tag{3}$$

where the self-energy Σ is given by

$$\Sigma(z)=z-\bar{\epsilon}-F(z). \tag{4}$$

Assuming, for the moment, that F is given by (2), we find for the spectral weight function

$$\begin{aligned}A(\mathbf{p},\omega)&=-2\,\mathrm{Im}G(\mathbf{p},\omega+i0^+)\\&=2\pi[Z_\mathbf{p}^-\delta(\omega-E_\mathbf{p}^-)+Z_\mathbf{p}^+\delta(\omega-E_\mathbf{p}^+)],\end{aligned} \tag{5}$$

where $E_\mathbf{p}^\pm$ are the two (real) roots of

$$E_\mathbf{p}^\pm=\epsilon_\mathbf{p}+\Sigma(E_\mathbf{p}^\pm), \tag{6}$$

and the renormalization coefficients $Z_p^\pm$ are given by

$$\begin{aligned}Z_\mathbf{p}^\pm&=\left[1-\frac{\partial}{\partial\omega}\Sigma(\omega)\right]^{-1}_{\omega=E_p^\pm}\\Z_\mathbf{p}^+&+Z_\mathbf{p}^-=1.\end{aligned} \tag{7}$$

Because the self-energy does not depend on wave vector p, we have the useful relation

$$\nabla_\mathbf{p}E_\mathbf{p}^\pm=Z_\mathbf{p}^\pm\nabla_\mathbf{p}\epsilon_\mathbf{p}. \tag{8}$$

We shall consider the case where the Fermi energy μ lies in the upper band of (5), and shall henceforth omit the "+" superscript from quantities referring to this band.

In a later paper,[4] Hubbard has refined his model to include the effects of "resonance broadening" and "scattering" corrections on the atomic resonance function $F(z)$. The spectral weight function thus obtained does not retain the simple structure of (5). However, there are still split bands, if the bandwidth is sufficiently small; roughly speaking, one replaces the δ functions of (5) with functions of finite width.

In this paper we consider not the equilibrium properties of Hubbard's model, but its behavior in crossed electric and magnetic fields,

$$\begin{aligned}e\mathbf{E}&=-\nabla U-(\partial/\partial T)\mathbf{K},\\e\mathbf{B}&=c\nabla\times\mathbf{K}.\end{aligned} \tag{9}$$

We describe the response of the system to the fields using the functions[20] $g^<(\mathbf{p},\omega;\,\mathbf{R},T)$ and $g^>(\mathbf{p},\omega;\,\mathbf{R},T)$, which, respectively, represent the numbers of particles and holes per atom with wave vector $\mathbf{p}$ and energy ω in the vicinity of the macroscopic space time point $\mathbf{R},T$. The total (local) numbers of electrons and holes per

[18] L. P. Kadanoff and G. Baym, *Quantum Statistical Mechanics* (W. A. Benjamin, Inc., New York, 1962), hereafter abbreviated KB. For a discussion of the equilibrium properties of the Green's functions we use, see also P. C. Martin and J. Schwinger, Phys. Rev. 115, 1342 (1959). For applications of the transport theory see R. E. Prange and L. P. Kandanoff, *ibid.* 134, A566 (1964), and also D. C. Langreth, Ph.D. thesis, University of Illinois, 1964 (unpublished). For a generalization of the KB equations to a solid, see B. L. Jones and J. M. McClure, Phys. Rev. 143, 133 (1966).

[19] In general, we follow the notation of KB (Ref. 18). Specifically, we pick units such that $\hbar$ and the volume of the system are unity. Notice that Hubbard's definition of the Green's function differs from KB's by a factor of 2π.

[20] See KB, Ref. 18, p. 60 and p. 102 for definitions of $g^\gtrless$. Note that in a solid the "spatial" coordinates become Wannier site indices.

atom is then[21]

$$n_e(\mathbf{R},T)=(2/2\pi)\sum_p \int d\omega\, g^<(\mathbf{p},\omega;\mathbf{R},T),$$
$$n_h(\mathbf{R},T)=(2/2\pi)\sum_p \int d\omega\, g^>(\mathbf{p},\omega;\mathbf{R},T), \quad (10)$$

and the current per atom is

$$\mathbf{j}(\mathbf{R},T)=(2e/2\pi)\sum_{\mathbf{p}} \int d\omega\, \nabla_{\mathbf{p}}\epsilon_{\mathbf{p}-\mathbf{K}} g^<(\mathbf{p},\omega;\mathbf{R},T). \quad (11)$$

For compactness we shall usually suppress the $\mathbf{R},T$ arguments, denoting nonequilibrium quantites by lower case letters, and their equilibrium analogs by capitals.

In terms of $g^<$ and $g^>$, the nonequilibrium Green's function g and spectral weight function a are given by

$$g(\mathbf{p},z)=\int \frac{d\omega}{2\pi}\frac{a(\mathbf{p},\omega)}{z-\omega}=\int\frac{d\omega}{2\pi}\frac{g^<(\mathbf{p},\omega)+g^>(\mathbf{p},\omega)}{z-\omega}. \quad (12)$$

The nonequilibrium Green's function has the same structure as the equilibrium one[22]:

$$g(\mathbf{p},z)=[z-\epsilon_{\mathbf{p}-\mathbf{K}}-U-\sigma(\mathbf{p},z)]^{-1}, \quad (13)$$

where

$$\sigma(\mathbf{p},z)=\sigma(\mathbf{p},\infty)+\int\frac{d\omega}{2\pi}\frac{\gamma(\mathbf{p},\omega)}{z-\omega}$$
$$=\sigma(\mathbf{p},\infty)+\int\frac{d\omega}{2\pi}\frac{\sigma^>(\mathbf{p},\omega)+\sigma^<(\mathbf{p},\omega)}{z-\omega}. \quad (14)$$

The quantities $\sigma^>(\mathbf{p},\omega)$ and $\sigma^<(\mathbf{p},\omega)$ defined by KB, represent, respectively, the scattering rate of an electron into the state $\mathbf{p}\omega$ given that it is originally unoccupied, and the scattering rate out of the state $\mathbf{p}\omega$ given that it is originally occupied. The sum of these rates $\gamma(\mathbf{p},\omega)$ is proportional to the inverse lifetime of the state. The (real) quantity $\sigma(\mathbf{p},\infty)$ is the part of the self-energy that is local in time.

For a complete description of the nonequilibrium properties of Hubbard's model, we would need a knowledge of the nonequilibrium values of the functions $\sigma^{\gtrless}$. For a calculation of the high-field Hall coefficient, however, we shall only need to use one property which $\sigma^{\gtrless}$ is assumed to have, which we describe below. In thermal equilibrium, the scattering rates are embodied in the function $F(z)$, which is independent of wave vector, because it represents the resonant properties of the individual localized atoms. Hence the equilibrium scattering rate functions $\Sigma^{\gtrless}$ are also independent of wave vector. The interatomic kinetic energy never gets renormalized. It is clear that if this same philosophy were carried out in a calculation of $\sigma^{\gtrless}$ for small deviations from equilibrium the insensitivity to wave vector would persist. Thus, following Hubbard, we henceforth neglect any wave-vector dependence that $\sigma^{\gtrless}$ may have. In fact, this wave-vector independence is the only property of Hubbard's model that we shall need, aside from the qualitative notion that there are two split bands. We never use any of the specific details of Hubbard's calculation.

III. THE HALL COEFFICIENT

In this section we consider only the simpler form of Hubbard's model. That is, we assume that the spectral weight function $a(\mathbf{p},\omega)$ has the structure depicted by Eqs. (5)–(8). These assumptions enable us to retain an analogy between Hubbard's model and a normal Fermi liquid. They will be relaxed in Sec. IV.

To determine $g^>$ and $g^<$ we use the Kadanoff-Baym equations[23] (KBE). These equations are expansions of the exact Green's-function equations in terms of the time and space derivatives of the external potentials $\mathbf{K}$ and U. We note that for Hubbard's model any change in the density of the particles involves a reshuffling of the populations of the upper and lower bands. Since the energy difference between the bands is the largest energy in the problem, the KB expansion is probably not appropriate. However, if we restrict ourselves to steady-state phenomena where only the characteristics of the upper band are changed then we may expect the KBE to give the linear response to the electric field and the semiclassical response to the magnetic field exactly.

The KBE for $g^<$ is

$$[\omega-U-\epsilon_{\mathbf{p}-\mathbf{K}}-\mathrm{Re}\sigma,\, g^<]_{p,\omega}+[\mathrm{Re}g,\sigma^<]_{p,\omega}=-\sigma^>g^<+\sigma^<g^>. \quad (15)$$

The equation for $g^>$ is obtained by interchanging all $>$'s and $<$'s in (15). The bracket notation on the left side of (15) means

$$[F,G]_{p,\omega}=\frac{\partial F}{\partial\omega}\frac{\partial G}{\partial T}-\frac{\partial F}{\partial T}\frac{\partial G}{\partial\omega}$$
$$-\nabla_p F\cdot\nabla_{\mathbf{R}}G+\nabla_{\mathbf{R}}F\cdot\nabla_p G \quad (16)$$

for any two functions F and G.

It is desirable to add some sort of dissipative mechanism to Hubbard's model, to give the system a finite conductivity. We do this by replacing the right side of (15) by

$$-(\sigma^>+\bar\sigma^>)g^<+(\sigma^<+\bar\sigma^<)g^>, \quad (17)$$

[21] In a solid, $n_e(\mathbf{R},T)$ does not strictly represent the electronic density, but rather the occupation number of the Wannier state centered at $\mathbf{R}$. In thermal equilibrium it is independent of R. Similar comments apply to n_h and $\mathbf{j}$. Equations (10) and (11) hold when the potentials U and $\mathbf{K}$ do not vary appreciably over a lattice spacing: they give the linear response to the electric field and semiclassical response to the magnetic field correctly.

[22] See KB, Ref. 18, p. 116.

[23] Reference 18, pp. 33 and 102.

where

$$\tilde{\sigma}^{\gtrless}(\mathbf{p},\omega;\,\mathbf{R},T)=\sum_{\mathbf{p}'} M_{\mathbf{p},\mathbf{p}'}g^{\gtrless}(\mathbf{p}',\omega;\,\mathbf{R},T).$$

The above interaction is typical of some elastic scattering mechanism. For example, for randomly positioned impurity centers interacting weakly with the electrons, it takes the form

$$M_{p,p'}=n_I\int d^3x\left|\int d^3r\,\varphi_p^*(\mathbf{r})V(\mathbf{r}-\mathbf{x})\varphi_{p'}(\mathbf{r})\right|^2, \quad (18)$$

where n_I is the impurity density, $V(\mathbf{r})$ the impurity potential, and φ_p the electronic Bloch functions. Since we only intend to treat these dissipative effects to lowest order, we need not modify the left side of (15).

The KBE may be expressed in a manifestly gauge-invariant, and more convenient form by regareing $\mathbf{P}$, Ω, $\mathbf{R}$, T as the independent variables instead of $\mathbf{p}$, ω, $\mathbf{R}$, T, where $\mathbf{P}=\mathbf{p}-\mathbf{K}(\mathbf{R},T)$, $\Omega=\omega-U(\mathbf{R},T)$. Then (16) becomes

$$[F,G]_{p,\omega}=[F,G]_{\mathbf{P},\Omega}+e\mathbf{E}\cdot\left(\frac{\partial F}{\partial\Omega}\nabla_{\mathbf{P}}G-\frac{\partial G}{\partial\Omega}\nabla_{\mathbf{P}}F\right)+\frac{e}{c}\mathbf{B}\cdot(\nabla_{\mathbf{P}}F\times\nabla_{\mathbf{P}}G). \quad (19)$$

In deriving (19) we have used, among others, the identities

$$\nabla_{\mathbf{R}}f[\mathbf{g}(\mathbf{R})]=\nabla_{\mathbf{g}}f\cdot\nabla_{\mathbf{R}}\mathbf{g}+\nabla_{\mathbf{g}}f\times(\nabla_{\mathbf{R}}\times\mathbf{g}),$$
$$\boldsymbol{\alpha}\cdot(\nabla\boldsymbol{\beta})\cdot\boldsymbol{\gamma}-\boldsymbol{\gamma}\cdot(\nabla\boldsymbol{\beta})\cdot\boldsymbol{\alpha}=-\boldsymbol{\gamma}\cdot\boldsymbol{\alpha}\times(\nabla\times\boldsymbol{\beta}). \quad (20)$$

As we show below, Eqs. (15) may be reduced to an ordinary Boltzmann-like equation with the ansatz

$$g^{<}(\mathbf{p},\omega;\,\mathbf{R},T)=a(\mathbf{P},\Omega)f_{\mathbf{P}}, \quad (21a)$$
$$g^{>}(\mathbf{p},\omega;\,\mathbf{R},T)=a(\mathbf{P},\Omega)(1-f_{\mathbf{P}}). \quad (21b)$$

Notice that we assume that $g^{<}$ and $g^{>}$, and hence all other quantities, depend on $\mathbf{R}$ and T only implicitly through the definition of $\mathbf{P}$ and Ω. Such a trial solution clearly satisfies our steady-state conditions that $n(\mathbf{R},T)$ and $\mathbf{j}(\mathbf{R},T)$ be independent of $\mathbf{R}$ and T, and we will find that it also satisfies the KBE. The utility of (19) is now immediately apparent, since in our case $[F,G]_{\mathbf{P},\Omega}=0$.

For Ω in the upper band, $\sigma^{>}$ and $\sigma^{<}$ vanish, so that in evaluating the left side of (15), we need only evaluate (19) with $F=\Omega-\epsilon_{\mathbf{P}}-\mathrm{Re}\sigma(\Omega)$ and $G=g^{<}(\mathbf{P},\Omega)=a(\mathbf{P},\Omega)f_{\mathbf{P}}$:

$$[(\Omega-\epsilon_{\mathbf{P}}-\mathrm{Re}\sigma),\,a(\mathbf{P},\Omega)f_{\mathbf{P}}]_{p,\omega}$$
$$=a(\mathbf{P},\Omega)[(\Omega-\epsilon_{\mathbf{P}}-\mathrm{Re}\sigma),f_{\mathbf{P}}]_{p,\omega}$$
$$=a(\mathbf{P},\Omega)\left[\left(1-\frac{\partial}{\partial\Omega}\mathrm{Re}\sigma\right)e\mathbf{E}\cdot\nabla_{\mathbf{P}}f_{\mathbf{P}}-\frac{e}{c}\mathbf{B}\cdot(\nabla_{\mathbf{P}}\epsilon_{\mathbf{P}}\times\nabla_{\mathbf{P}}f_{\mathbf{P}})\right]. \quad (22)$$

The first equality above follows because $a(\mathbf{P},\Omega)=2\pi\delta(\Omega-\epsilon_{\mathbf{P}}-\mathrm{Re}\sigma)$ "commutes" with $\Omega-\epsilon_{\mathbf{P}}-\mathrm{Re}\sigma$. Because of the vanishing of $\sigma^{\gtrless}$ the evaluation of the right side (15) of the KBE is straightforward. Finally an Ω integration over the upper band yields

$$[e\mathbf{E}+(e/c)\nabla_{\mathbf{P}}e_{\mathbf{P}}\times\mathbf{B}]\cdot\nabla_{\mathbf{P}}f_{\mathbf{P}}=-2\pi\sum_{\mathbf{P}'}z_{\mathbf{P}}M_{\mathbf{P},\mathbf{P}'}z_{\mathbf{P}'}\delta(e_{\mathbf{P}}-e_{\mathbf{P}'})[f_{\mathbf{P}}-f_{\mathbf{P}'}], \quad (23)$$

where $e_{\mathbf{P}}$ and $z_{\mathbf{P}}$ are defined analogously to their equilibrium counterparts, $E_{\mathbf{p}}$ and $Z_{\mathbf{P}}$. Similarly, one can easily verify that the substitution of (21b) into the KBE for $g^{>}$ yields (23) also. This redundancy of the second KBE simply means that the assumed structure of the solution was correct.

Equation (23) is, of course, aside from several renormalizations, just the independent-particle Boltzmann equation, which with certain assumptions about the form of $e_{\mathbf{P}}$, $M_{\mathbf{P},\mathbf{P}'}$, and $z_{\mathbf{P}}$ may be solved for the conductivity tensor. If we take $\mathbf{E}$ and $\mathbf{B}$ perpendicular, however, the right side of (23) plays no role in the high-B limit, and we henceforth neglect it. We have included it thus far to show that it leads to no unusual effects.

We linearize the left side of (23) in the electric field by letting

$$f_{\mathbf{P}}=F_{\mathbf{P}}+\delta f_{\mathbf{P}},\quad e_{\mathbf{P}}=E_{\mathbf{P}}+\delta E_{\mathbf{P}}, \quad (24)$$

where $F_{\mathbf{P}}$ and $E_{\mathbf{P}}$ are appropriate to thermal equilibrium (no fields). Then

$$-e\mathbf{E}\cdot\nabla_{\mathbf{P}}E_{\mathbf{P}}\delta(E_{\mathbf{P}}-\mu)-(e/c)\nabla_{\mathbf{P}}E_{\mathbf{P}}\cdot(\nabla_{\mathbf{P}}\delta E_{\mathbf{P}}\times\mathbf{B})\times\delta(E_{\mathbf{P}}-\mu)+(e/c)(\nabla_{\mathbf{P}}E_{\mathbf{P}}\times\mathbf{B})\cdot\nabla_{\mathbf{P}}\delta f_{\mathbf{P}}=0. \quad (25)$$

A solution[24] of (25) is (recalling that $\mathbf{E}\perp\mathbf{B}$)

$$\delta f_{\mathbf{P}}=[cB^{-3}\mathbf{P}\cdot(\mathbf{E}\times\mathbf{B})-\delta E_{\mathbf{P}}]\delta(E_{\mathbf{P}}-\mu). \quad (26)$$

Equation (23) is actually quite general. The only assumption needed in its derivation was that $\sigma^{>}$ and $\sigma^{<}$ vanished at and were continuous across the Fermi surface. Thus (26) is valid for a normal Fermi liquid as well.[25] The main problem in its general application is to express the current in terms of $\delta f_{\mathbf{P}}$, and to calculate $\delta E_{\mathbf{P}}$, if necessary. For a normal Fermi liquid, the current is given by[25]

$$\mathbf{j}=2e\sum_{\mathbf{P}}(\nabla_{\mathbf{P}}e_{\mathbf{P}})f_{\mathbf{P}}\rightarrow 2e\sum_{\mathbf{P}}\nabla_{\mathbf{P}}E_{\mathbf{P}}[\delta f_{\mathbf{P}}+\delta E_{\mathbf{P}}\delta(E_{\mathbf{P}}-\mu)]$$
$$=2ecB^{-2}\sum_{\mathbf{P}}(\nabla_{\mathbf{P}}E_{\mathbf{P}})\mathbf{P}\cdot(\mathbf{E}\times\mathbf{B})\delta(E_{\mathbf{P}}-\mu). \quad (27)$$

Hence the Hall coefficient is given by

$$(ecR)^{-1}=\frac{2}{(2\pi)^3}\frac{1}{3}\int_{\text{Fermi surface}}\mathbf{P}\cdot\mathbf{n}dS, \quad (28)$$

where $\mathbf{n}$ is a unit normal vector in the direction of $\nabla_{\mathbf{P}}E_{\mathbf{P}}$. We assume that the holes occupy closed regions

[24] Equation (19) determines $\delta f_{\mathbf{P}}$ to within an additive function of $E_{\mathbf{P}}$, which does not affect the current.

[25] See KB, Ref. 18, Chap. 11.

of momentum space, so that (28) becomes

$$(ecR)^{-1}=-2V/(2\pi)^3, \tag{29}$$

where V is the volume of momentum space (per zone) occupied by the holes. Of course, in normal systems, $2V/(2\pi)^3$ is just the density of holes, so that compensation results.

In Hubbard's model, we may calculate the current using (11) and (21) plus the nonequilibrium analogs of (5) and (8):

$$\begin{aligned}\mathbf{j}&=2e\sum_{\mathbf{p}}\int(d\Omega/2\pi)(\nabla_{\mathbf{p}}\epsilon_{\mathbf{p}})a(\mathbf{P},\Omega)f_{\mathbf{p}}\\&=2e\sum{}_{\mathbf{p}}z_{\mathbf{p}}(\nabla_{\mathbf{p}}\epsilon_{\mathbf{p}})f_{\mathbf{p}}=2e\sum{}_{\mathbf{p}}(\nabla_{\mathbf{p}}\epsilon_{\mathbf{p}})f_{\mathbf{p}},\end{aligned} \tag{30}$$

so that (29) is valid in this case as well.[26] However, $2V/(2\pi)^3$ is greater than the density of holes, since

$$n_h=2\sum_{E_{\mathbf{p}}>\mu}Z_{\mathbf{p}},\quad 0<Z_{\mathbf{p}}<1, \tag{31}$$

so that Hubbard's model does not predict compensation.

IV. EXTENSION TO INCLUDE LIFETIME EFFECTS

Here we generalize the results of the preceding section. As noted earlier, Hubbard's more sophisticated model[4] does not retain the property of vanishing widths (Γ), so that the arguments of the preceding section do not apply. Of course, the wave-vector independence of the self-energy does persist; fortunately this is the only property we shall need in the high-field limit.

The ansatz (21) no longer holds. Nevertheless, we may linearize the terms in the electric field on the left side of the KBE using the local equilibrium values

$$\begin{aligned}g^<(\mathbf{P},\Omega)&=A(\mathbf{P},\Omega)[1-\theta(\Omega-\mu)],\\g^>(\mathbf{P},\Omega)&=A(\mathbf{P},\Omega)\theta(\Omega-\mu),\\\sigma^<(\Omega)&=\Gamma(\Omega)[1-\theta(\Omega-\mu)],\\\sigma^>(\Omega)&=\Gamma(\Omega)\theta(\Omega-\mu).\end{aligned} \tag{32}$$

According to (15) then, we must evaluate the second term of (19) with $F=\Omega-\epsilon_{\mathbf{p}}-\mathrm{Re}\sigma$, $G=g^<$, and add it to the evaluation with $F=\mathrm{Re}g$, $G=\sigma^<$, where $g^\lessgtr$ and $\sigma^\lessgtr$ are given by (32). This evaluation is a matter of straightforward algebra; using Eqs. (12)–(14) plus the wave-vector independence of the self-energy, one obtains

$$-e\mathbf{E}\cdot\nabla_{\mathbf{p}}\epsilon_{\mathbf{p}}Q(\epsilon_{\mathbf{p}},\Omega)2\pi\delta(\Omega-\mu), \tag{33}$$

where

$$Q(\epsilon_{\mathbf{p}},\Omega)=\Gamma(\Omega)A^2(\mathbf{P},\Omega)/4\pi. \tag{34}$$

To evaluate the terms on the left side of (15) proportional to the magnetic field, we must evaluate the last term of (19). Here we cannot use (32); however, the wave-vector independence of $\sigma^\lessgtr$ leads to considerable simplification. We obtain

$$(e/c)(\nabla_{\mathbf{p}}\epsilon_{\mathbf{p}}\times B)\cdot\nabla_{\mathbf{p}}g^<(\mathbf{P},\Omega). \tag{35}$$

Thus the KBE (15) becomes

$$\begin{aligned}&-e\mathbf{E}\cdot\nabla_{\mathbf{p}}\epsilon_{\mathbf{p}}Q(\epsilon_{\mathbf{p}},\Omega)2\pi\delta(\Omega-\mu)\\&\quad+(e/c)(\nabla_{\mathbf{p}}\epsilon_{\mathbf{p}}\times B)\cdot\nabla_{\mathbf{p}}g^<(\mathbf{P},\Omega)\\&\quad=-\sigma^>(\mathbf{P},\Omega)g^<(\mathbf{P},\Omega)+\sigma^<(\mathbf{P},\Omega)g^>(\mathbf{P},\Omega).\end{aligned} \tag{36}$$

Again we assume $\mathbf{E}\perp\mathbf{B}$ and take the high-B limit,[27] so that the terms on the right side of (36) may be neglected. Then (36) has a trivial solution, which, when combined with (11) gives

$$\mathbf{j}=2ecB^{-2}\textstyle\sum_{\mathbf{p}}(\nabla_{\mathbf{p}}\epsilon_{\mathbf{p}})(\mathbf{E}\times\mathbf{B})\cdot\mathbf{P}Q(\epsilon_{\mathbf{p}},\mu). \tag{37}$$

Assuming again that the holes occupy closed regions in momentum space, we find

$$-(ecR)^{-1}=\int d\epsilon\,Q(\epsilon,\mu)[2V(\epsilon)/(2\pi)^3], \tag{38}$$

where $V(\epsilon)$ is the volume of momentum space enclosed by the surface $\epsilon_{\mathbf{p}}=\epsilon$.

Note that $Q(\epsilon,\mu)$, when considered as a function of ϵ, is peaked around $\epsilon=\mu-\Sigma(\mu)$, has unit area, and width $\sim\Gamma(\mu)$. Thus as $\Gamma(\mu)\to 0$, we recover the results of Sec. III. Even in the more general case $\Gamma(\mu)\neq 0$, however, $(ecR)^{-1}$ is proportional to an average momentum space volume, and not to the hole density. We emphasize that none of the details of Hubbard's model have been used in the calculation; Eq. (38) follows solely from the wave-vector independence of the self-energy functions.

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[26] We have tacitly assumed that with μ in the upper band, the lower band contributes nothing to the current. This may be seen by repeating the steps leading to Eq. (23) for the lower band, thus deriving an identical equation. When this equation for the lower band is linearized in $\mathbf{E}$, then one finds that the change in the distribution function is proportional to $\delta(E_{\mathbf{p}^-}-\mu)$, which is zero by assumption.

[27] We should point out that unless the bandwidth is small enough so that the bands are well separated, $\sigma^\lessgtr$ would be too large for this high-field limit to be attainable in practice.