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Hall Effect in the Presence of Strong Spin-Disorder Scattering

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The Hall mobility μ_H of a single hole in a Mott-Hubbard band of a magnetic insulator is considered using a path formulation of the atomic limit of the Hubbard model. It is shown that within a generalization of the retraceable-path approximation, the Hall mobility and the drift mobility μ_D are essentially equal at high temperatures compared with the bandwidth, but that the Hall mobility becomes small compared to the drift mobility as the temperature is lowered. The ratio μ_H/μ_D becomes proportional to the ratio of the temperature to the bandwidth at low temperatures.

I. INTRODUCTION

The theory of the Hall effect in the presence of strong scattering is a difficult problem. A general discussion of the problem has been given by Herring[1] and by Kubo.[2] The specific cases of liquid metals have been examined by Springer[3] and by Allgaier[4] and of small polarons by Friedman and Holstein[5] and by Emin and Holstein.[6] In this paper we shall examine the case of an electron or hole in a magnetic semiconductor which is strongly coupled to and scattered by spin waves. An excellent and detailed review of the experimental situation in magnetic semiconductors such as NiO, CoO, Fe_2O_3, and MnO has been given recently by Bosman and van Daal.[7] These authors conclude that the free carriers in most of these materials are probably not small polarons and they point out the importance of a theoretical understanding of transport properties and in particular the Hall effect in the presence of strong spin-disorder scattering.

In this paper we shall examine the Hall effect for an extra carrier (electron or hole) in an otherwise half-filled band in the atomic limit of the Hubbard model. Langreth[8] has examined the Hall coefficient using Hubbard's approximate treatment of his model.[9] However, this treatment ignores the strong coupling between an extra carrier and the localized spins. This coupling is so strong in the atomic limit that as shown recently by Ohata and Kubo[10] and by the present authors,[11] the motion of an extra carrier is more properly considered as a diffusion or Brownian motion through the lattice rather than a propagating or wavelike motion. The former authors calculated the first few moments of the frequency-dependent conductivity and by fitting a Gaussian or a Lorentzian form to the conductivity-obtained values for the dc mobility. The latter authors used a technique due to Nagaoka[12] of representing the problem in terms of walks on a lattice to examine the density of states for the extra carrier. They found that an approximation in which only walks with no closed loops are included gave a very reasonable form for the density of states in

the bulk of the band. This approximation can also be obtained using Green's functions by replacing the infinite hierarchy of equations by a recurrence relation.[13] The dc mobility was also calculated within this approximation[11] and the values obtained agree well with those of Ohata and Kubo.[10] These values for the mobility are quite low, indicating that the motion is primarily diffusive.

The calculation of the Hall coefficient is considerably more difficult than that of the dc mobility. The moments of the antisymmetric part of the conductivity transverse to the magnetic field $[\sigma^a_{xy}(\omega)]$ give information about its imaginary part whereas the Hall coefficient is related to the real part. By assuming a form for the imaginary part of $\sigma^a_{xy}(\omega)$ we can obtain an approximate value for the Hall coefficient at high temperatures. The Hall effect arises from paths which enclose a finite area transverse to the magnetic field so that, within the approximation of summing only paths with no closed loops used previously by the present authors, the Hall mobility is identically zero. An extension of this approximation wherein walks on a square are dressed with all possible walks with no closed loops, however, gives a finite Hall effect. We shall calculate the Hall mobility using this approximation. The result agrees well with the values deduced from the exact moments at high temperatures and is almost equal to the drift mobility. At lower temperatures the values for the Hall mobility μ_H are considerably smaller than that calculated previously for the drift mobility μ_D. However our results for μ_H are clearly more suspect than those we found for μ_D. It is possible that the inclusion of higher-order terms could change the values obtained substantially. Nonetheless, it is clear from this work that μ_D and μ_H are not simply related in the presence of strong spin-disorder scattering and can differ substantially.

The model considered here ignores the influence of spin-orbit coupling on the Hall effect. This effect has been investigated by several authors[14] and is known to give rise to the anomalous Hall coefficient in ferromagnets. We shall restrict ourselves to paramagnetic materials where Maranzana[15] has found that such contributions are small.

In Sec. II we shall derive the necessary formalism and discuss the moment calculation. In Sec. III we will evaluate the Hall coefficient within the approximation of including walks on a square dressed with the walks with no closed loops. Finally, in Sec. IV, we discuss the relationship of our work to that of Mott[16] and Cohen[17] on the form of the mobility near the mobility edge in disordered semiconductors.

II. MOMENT TECHNIQUE

The Hubbard model Hamiltonian[9] has the form

$$H=\sum_{ij\sigma} t_{ij}\, c^\dagger_{i\sigma} c_{j\sigma} + U\sum_i n_{i\uparrow} n_{i\downarrow}\ , \tag{1}$$

where $c^\dagger_{i\sigma}$ is the creation operator for an electron with spin σ in the Wannier state localized at the site i and $n_{i\sigma}(\equiv c^\dagger_{i\sigma} c_{i\sigma})$ is the number operator for electrons with spin σ at the site i. The first term represents the hopping from site j to i and we shall consider the case where t_{ij} is nonzero only for i and j nearest neighbors. The second term represents the intra-atomic Coulomb interaction. We shall restrict ourselves to the case where there is an extra hole (or electron) in an otherwise half-filled band in the atomic limit where $t_{ij}(\equiv t)$ is finite but $U\to\infty$. In this limit we can replace the Hamiltonian (1) by an effective Hamiltonian of the form

$$H'=\sum_{in\sigma} c^\dagger_{i+n\sigma} c_{i\sigma} P, \tag{2}$$

where n denotes the nearest neighbors of i, and P is a projection operator such that $P=1$ operating on a state with one hole and $P=0$ otherwise.

In the presence of a magnetic field the Wannier states $\chi(\vec{\mathbf{r}}-\vec{\mathbf{R}}_i)$ satisfy the equation

$$\left[\frac{1}{2m}\left(\vec{\mathbf{p}}+\frac{e}{c}\vec{\mathbf{A}}\right)^2+V(\vec{\mathbf{r}})\right]\chi(\vec{\mathbf{r}}-\vec{\mathbf{R}}_i)=\sum_j t_{ij}\chi(\vec{\mathbf{r}}-\vec{\mathbf{R}}_j), \tag{3}$$

where $\vec{\mathbf{p}}\equiv -i\vec{\nabla}$, $\vec{\mathbf{A}}$ is the vector potential, and V is the crystal potential ($\hbar=1$). We shall use a gauge in which

$$\vec{\mathbf{A}}=\tfrac{1}{2}(\vec{\mathcal{H}}\times\vec{\mathbf{r}}), \tag{4}$$

where $\vec{\mathcal{H}}$ is external magnetic field. It is straightforward to show[5] that to terms of order $\mathcal{H}^2$ we can work with the original Wannier states by modifying the matrix elements t_{ij} by the Peierls phase factor

$$t_{ij}\to t'_{ij}=t_{ij}\, e^{i\vec{\mathcal{H}}\cdot(\vec{\mathbf{R}}_j\times\vec{\mathbf{R}}_i)(e/2c)}\ . \tag{5}$$

We shall consider only a simple-cubic lattice with the magnetic field oriented along the z direction. The current operators in the xy plane take the form

$$J_x=iea\sum_{i\sigma}\left(t'_{i+x,i}\, c^\dagger_{i+x,\sigma} c_{i\sigma} - t'_{i-x,i}\, c^\dagger_{i-x,\sigma} c_{i,\sigma}\right), \tag{6}$$

$$J_y=iea\sum_{i\sigma}\left(t'_{i+y,i}\, c^\dagger_{i+y,\sigma} c_{i\sigma} - t'_{i-y,i}\, c^\dagger_{i-y,\sigma} c_{i\sigma}\right), \tag{7}$$

where e is the electronic charge and a the lattice parameter. The low-field Hall mobility μ_H is defined as

$$\mu_H=\lim_{\mathcal{H}\to 0}\lim_{\omega\to 0}\frac{c}{\mathcal{H}}\,\frac{\sigma_{yx}(\mathcal{H},\omega)}{\sigma_{xx}(\mathcal{H},\omega)}\ , \tag{8}$$

where c denotes the velocity of light. The conductivities σ_{yx} and σ_{xx} may be calculated from the Kubo formula[2]

$$\sigma_{\alpha\beta}(\omega)=\frac{1}{Z\Omega}\int_0^\infty d\tau\int_0^\beta d\lambda\ \mathrm{Tr}[\zeta_0 J_\alpha(0) J_\beta(\tau+i\lambda)]\, e^{-i\omega\tau}, \tag{9}$$

where $\zeta_0(\equiv e^{-\beta H'})$ is the density matrix, Ω is the vol-

ume of the system, Z is the partition function for a single hole, and $\beta = 1/k_B T$. The trace in Eq. (9) is to be taken over all states with a single hole and arbitrary spin configurations. Now the eigenstates of the Hamiltonian H' lie between $\pm zt$ so we may conveniently introduce the resolvant operators of the exponential operators and perform the τ and λ integrals to obtain the result

$$\sigma_{\alpha\beta}(\omega) = \frac{-i}{Z\Omega}\int_{C_1}\frac{d\omega_1}{2\pi i}\int_{C_1}\frac{d\omega_2}{2\pi i}\,\frac{1}{\omega-\omega_2+\omega_1} \times \frac{e^{-\beta\omega_2}-e^{-\beta\omega_1}}{\omega_1-\omega_2}\,\mathcal{F}_{\alpha\beta}(\omega_1,\omega_2), \quad (10)$$

where the contour C_1 encloses the region $-zt<\omega<zt$ on the real axis. The function $\mathcal{F}_{\alpha\beta}(\omega_1,\omega_2)$ is defined as

$$\mathcal{F}_{\alpha\beta}(\omega_1,\omega_2) = \mathrm{Tr}\left\langle \frac{1}{\omega_1-H'}\,J_\alpha\,\frac{1}{\omega_2-H'}\,J_\beta\right\rangle . \quad (11)$$

The corrections to σ_{xx} are of order $\mathcal{K}^2$ and so can be neglected in Eq. (8). The calculation of the Hall mobility therefore reduces to a calculation of the term in the transverse conductivity which is linear in $\mathcal{K}$. This term is antisymmetric in x and y and it is more convenient to calculate with the explicitly antisymmetric function $\sigma^a_{xy} = \frac{1}{2}(\sigma_{xy}-\sigma_{yx})$.

In order to calculate moments we must consider the complete function σ^a_{xy} at large ω and expand it as a power series in $1/\omega$. Let us write

$$\sigma^a(\omega) = \frac{1}{Z}\sum_{n=2}^{\infty}\sum_{m=2}^{\infty} A_{n,m}\,\frac{\beta^m}{\omega^n} . \quad (12)$$

To obtain the coefficients A_{nm} we must expand $\mathcal{F}^a(\omega_1,\omega_2)\,[\equiv\frac{1}{2}(\mathcal{F}_{xy}-\mathcal{F}_{yx})]$ as a power series in $(1/\omega_{1,2})$ for large values of ω_1,ω_2. The leading term is of order $(\omega_{1,2})^{-4}$ and we shall denote it by $\mathcal{F}^a_4$:

$$\mathcal{F}^a_H = \frac{1}{\omega_1\omega_2}\,\mathrm{Tr}\left\langle \frac{H'^2}{\omega_1^2}\,(J_xJ_y-J_yJ_x) + \frac{1}{\omega_1\omega_2}\,(H'J_xH'J_y-H'J_yH'J_x) + \left(J_x\frac{H'^2}{\omega_2^2}J_y - J_y\frac{H'^2}{\omega_2^2}J_x\right)\right\rangle . \quad (13)$$

The second term is identically zero by the cyclic property of the trace. The first and third terms may be combined to give

$$\mathcal{F}^a_4 = \frac{1}{\omega_1\omega_2}\left(\frac{1}{\omega_1^2}-\frac{1}{\omega_2^2}\right)\,\mathrm{Tr}\langle H'^2(J_xJ_y-J_yJ_x)\rangle . \quad (14)$$

To evaluate the trace in Eq. (14) we must sum over the number of paths for the hole in which the hole returns to origin after exactly four steps. The directions of the initial two steps are determined by the J_x and J_y operators. We must carefully add up the Peierl's phase in the hopping matrix elements. When the hole moves around a closed square in four steps, the phase factors in (5) add up to give a net phase factor of

$$e^{i(e/c)\vec{\mathcal{H}}\cdot\vec{a}_{1234}} = \exp[i(e/c)\vec{\mathcal{H}}\cdot\tfrac{1}{2}(\vec{R}_1\times\vec{R}_2+\vec{R}_2\times\vec{R}_3+\vec{R}_3\times\vec{R}_4+\vec{R}_4\times\vec{R}_1)] = e^{\pm i\varphi}, \quad (15)$$

where $\varphi = ea^2\mathcal{H}/c$ and the positive sign is for paths in the clockwise direction and the negative sign is for paths in the anticlockwise direction. For a path which does not involve a closed loop the sum entering the phase factor is identically zero and such paths will not contribute to the trace (14). In general, the exponent of the phase factor is proportional to the area of the closed loop and all paths with no closed loops will give no contribution to $\mathcal{F}^a$. In evaluating the contribution to the average (14) we need consider only paths where the hole circumscribes a square. We must take account in which direction the hole circumscribes the square since this will determine the sign of the phase factor. Using (7) and (15) we arrive at the result

$$\mathcal{F}^a_4 = -8ie^2a^2t^4\sin\varphi\,\frac{r}{\omega_1\omega_2}\left(\frac{1}{\omega_1^2}-\frac{1}{\omega_2^2}\right), \quad (16)$$

where r is the probability that the three spins at the vertices of the square are aligned. (If the spins are not aligned, then the final spin configuration is different from the starting spin configuration and the path is not an allowed one.) The value of r will depend on the spin configuration. We will restrict ourselves in this paper to a random arrangement of the spins for which $r=\frac{1}{4}$.

After substituting Eq. (16) into Eq. (10), the contour integrals can be performed at once, and we arrive at the result for the coefficient $A_{2,2}$:

$$A_{2,2} = -8(e^3a^4t^4\mathcal{H}/c)r. \quad (17)$$

In a similar way we can evaluate the higher coefficients $A_{2,4}$ and $A_{4,2}$. Expanding Eq. (11) to terms of order $\omega_{1,2}^{-6}$ we obtain

$$\mathcal{F}^a_6 = \left(\frac{1}{\omega_1^5\omega_2}-\frac{1}{\omega_1\omega_2^5}\right)\langle H'^4J_xJ_y-H'^4J_yJ_x\rangle + \left(\frac{1}{\omega_1^2\omega_2^4}-\frac{1}{\omega_1^4\omega_2^2}\right)\langle H'J_xH'^3J_y-H'J_yH'^3J_x\rangle . \quad (18)$$

The evaluation of the averages in Eq. (18) is described in the Appendix. Keeping only the terms linear in $\mathcal{H}$ we find for a random spin configuration

$$\mathcal{F}^a_6 = -ie^2a^2t^6\left(\frac{a^2e\mathcal{H}}{c}\right)\left[\frac{33}{\omega_1\omega_2}\left(\frac{1}{\omega_1^4}-\frac{1}{\omega_2^4}\right)-\frac{9}{\omega_1^2\omega_2^2}\left(\frac{1}{\omega_1^2}-\frac{1}{\omega_2^2}\right)\right]. \quad (19)$$

Substituting back in Eq. (10) and performing the contour integrals, we arrive at the result that

$$A_{2,4}/A_{2,2}=\tfrac{33}{24}\,t^2 \tag{20}$$

and

$$A_{4,2}/A_{2,2}=\tfrac{15}{2}\,t^2. \tag{21}$$

Using these moments, an estimate can be made of the value of $\sigma^a_{xy}(\omega)$ at $\omega=0$ to order $(zt/k_BT)^2$. First, we consider that $\sigma^a_{xy}(\omega)$ to order β^2 is of the form

$$\sigma^a_{xy}=-\int\frac{\omega' F(\omega')}{\omega-\omega'}d\omega' , \tag{22}$$

where $F(\omega')$ is a symmetric function of ω'. If we are interested in σ^a_{xy} to order β^2 then $A_{2,2}$ and $A_{4,2}$ represent the second and fourth moments of $F(\omega)$. Clearly, the dc value of σ^a_{xy} is the average value of $F(\omega)$. If we assume F is a Gaussian function, then we can fit the two known moments and deduce a value of $\sigma^a_{xy}(0)$. In this way we obtain

$$\sigma^a_{xy}(\omega=0)\simeq+4e^3a^4t^2\mathcal{H}/5c(k_BT)^2 . \tag{23}$$

This result will be used to evaluate the approximate treatment of the Hall mobility in Sec. III.

III. RETRACEABLE-PATH APPROXIMATION

In this section σ^a_{xy} will be estimated by considering the contribution from walks on the square but allowing all possible side excursions which start and finish at the same vertex on the square and in which all steps in the excursion are eventually retraced.[11] A few simple paths of this type are illustrated in Fig. 1. Summing such paths was considered extensively in the previous paper by the authors. There it was argued that this summation gives a reasonable estimate for the density of states in the bulk of the band for the extra hole. Here we assume that this same approximation will give a rough estimate of the Hall effect in the region of energy where the density of states is large.

Summing the retraced side excursions is equivalent to renormalizing each of the vertices of the simple square considered in Sec. II. One must, however, be careful not to double-count graphs. Thus, on the side of the square connected by the H' operators, after summing all retraceable paths originating from the first vertex next to the current operator, one must not include paths which immediately return to this vertex in renormalizing the second vertex. Likewise, for the renormalization of the third vertex one must not sum paths returning to the second. Using this argument $\mathcal{F}_a(\omega_1,\omega_2)$ is seen to be given by Eq. (16) with

$$\frac{1}{\omega_1\omega_2}\,\frac{1}{\omega_1^2}-\frac{1}{\omega_2^2}\;\to G(\omega_1)G(\omega_2)\left(\frac{1}{\{\omega_1[1-\Sigma_A(\omega_1)]\}^2}-\frac{1}{\{\omega_2[1-\Sigma_A(\omega_2)]\}^2}\right), \tag{24}$$

where

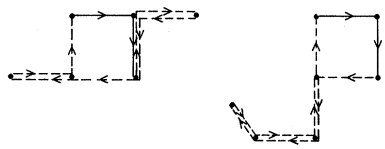

FIG. 1. An illustration of a few typical graphs with retraceable paths which renormalize the basic square in Sec. II.

$$G(\omega)=\omega\left[1-\frac{z}{(z-1)}\,\Sigma_A(\omega)\right]^{-1} \tag{25}$$

and

$$\Sigma_A(\omega)=\tfrac{1}{2}\left\{1-\left[1-\frac{4(z-1)}{\omega^2}\,t^2\right]^{1/2}\right\} . \tag{26}$$

The $G(\omega)$ represents the sum of all retraceable paths which return to the starting site whereas $\{\omega[1-\Sigma_A(\omega)]\}^{-1}$ sums only the forward going paths.[11] The small z is the coordination number of the lattice ($z=6$ in the simple-cubic lattice used here). In order to evaluate the Hall mobility we must perform the integrals in Eq. (10) and take the limit $\omega\to0$. One of these integrals can be performed analytically to give

$$\sigma^a_{xy}(\omega)=\frac{-i}{\Omega 2\omega Z}\int\frac{d\omega_1}{2\pi i}\,e^{-\beta\omega_1}\times[\mathcal{F}_a(\omega_1-\omega,\omega_1)-\mathcal{F}_a(\omega_1+\omega,\omega_1)] . \tag{27}$$

Substituting Eq. (24) for $\mathcal{F}_a$ and taking the limit $\omega\to0$ we obtain

$$\sigma^a_{xy}(\omega=0)=\frac{e^3a^4t^2 2\mathcal{H}}{\Omega cZ}\int_{-\infty}^{\infty}\frac{d\omega_1}{\pi}\,e^{-\beta\omega_1}\times\left(\mathrm{Im}[G(\omega_1)\alpha^{-2}(\omega_1)]\frac{d}{d\omega_1}\,\mathrm{Re}G(\omega_1)-\mathrm{Im}G(\omega_1)\frac{d}{d\omega_1}\,\mathrm{Re}[G(\omega_1)\alpha^{-2}(\omega_1)]\right) . \tag{28}$$

Here $\alpha(\omega)=\omega[1-\Sigma_A(\omega)]$ and the functions are evaluated just above the real axis. Substituting the expressions for G and α we obtain

$$\sigma^a_{xy}(\omega=0)=\frac{-4e^3a^4\mathcal{H}}{\Omega\omega_0\pi cZz}\int_{-\omega_0}^{\omega_0}d\bar{\omega}\,e^{-(\beta zt)\bar{\omega}}\times\frac{[1-(z-1)\bar{\omega}^2][1-(\bar{\omega}/\omega_0)^2]^{1/2}}{(1-\bar{\omega}^2)^2} , \tag{29}$$

where $\omega_0^2=4(z-1)/z^2$. We can now evaluate this final integral in two limits. In the first case with $k_BT\gg zt$ we find that

$$\sigma_{xy}=\frac{e^3a^4\mathcal{H}}{30c}\left(\frac{zt}{k_BT}\right)^2 . \tag{30}$$

Using Eq. (3.14) of our previous paper for the drift

mobility,[11] the high-temperature Hall mobility is found to be

$$\mu_H = 0.224ea^2 \frac{zt}{k_B T} . \tag{31}$$

If $a = 3$ Å,

$$\mu_H = 0.3 \frac{zt}{k_B T} \text{ cm}^2/\text{V sec}, \tag{32}$$

which is a value very close to the drift mobility $\sim 0.2(zt/k_B T)$ cm^2/V sec. It should be noted that Eq. (30) differs from the value obtained in Sec. II only by a factor of 1.5, which is some indication that our approximation is quite good in this regime. In fact, if we use the moments of the approximate $\sigma_{xy}(\omega)$ of Eq. (24), we find that the Gaussian technique underestimates $\sigma_{xy}(0)$ by a factor of 3. Therefore, Eq. (30) is probably a fairly accurate estimate of the high-temperature value.

For $k_B T \ll zt$ we expand the integrand in Eq. (29) about $\omega = -\omega_0$. The partition function

$$Z = \int_{-\omega_0 zt}^{\omega_0 zt} \frac{d\omega}{\pi} e^{-\beta\omega} \operatorname{Im} G(\omega - i\delta)$$

must also be expanded and the net result is that σ_{xy} becomes a constant

$$\sigma_{xy} = 8e^3 a^4 \mathcal{H} (5)^{1/2}/15c . \tag{33}$$

The Hall mobility is obtained from this by dividing by the drift mobility which was calculated in Ref. 11 but incorrectly printed there for $k_B T \ll zt$

$$\mu_D = [ea^2 4z/(z-2)^2][(z-1)^{1/2}/z\pi]^{1/2}(zt/k_B T)^{1/2}, \tag{34}$$

so that

$$\mu_H = ea^2 [\tfrac{32}{45} (6\pi)^{1/2}] (k_B T/zt)^{1/2} . \tag{35}$$

Thus, the Hall mobility is smaller than the drift mobility by a factor of $k_B T/zt$. This is an interesting result in light of the fact that NiO and other magnetic materials show Hall mobilities that are smaller than the drift mobility.[7]

IV. DISCUSSION

In this paper we have calculated the Hall mobility of an extra carrier in a magnetic insulator using a path formulation of the atomic limit of the Hubbard model. At high temperatures compared to the bandwidth the calculated Hall and drift mobilities agree, whereas at temperatures small compared with the bandwidth, the Hall mobility is smaller than the drift mobility by a factor of $k_B T/zt$. By comparing with the moment calculation it was argued in Sec. III that the calculated high-temperature Hall mobility appears to be fairly accurate. There is no such argument for the validity of the low-temperature Hall mobility and the calculation presented here should be regarded as a first attempt. However, it should be pointed out that the results obtained for low temperatures are similar to those proposed by Cohen[17] and Mott[16] for the so-called "Brownian motion" regime of disordered systems. In this regime the mean free path of the particle is of the order of the interatomic spacing. The energy-dependent drift mobility is thus proportional to the hopping integral squared times the density of states at a single site. In Ref. 11 it was shown that the spin-disorder scattering in the Hubbard model gives rise to precisely this form for the drift mobility. Friedman and Holstein[5] have calculated the Hall mobility for small polarons and found that the Hall conductivity depends on a three-site coincidence, so that the Hall mobility is proportional to the square of the density of states on a single site. This result is not exactly reproduced in the present calculation. Our result is written in terms of single-site propagators, but these propagators depend on the position along the path because only forward going paths are included. The three-site coincidence result of Friedman and Holstein[5] depends on the equivalence of the propagators along the path. Nevertheless, in the region near the edge of the band, the Hall mobility is proportional to the square of the density of states as in the polaron problem. This is the reason that the ratio μ_H/μ_D is proportional to $k_B T/zt$ at low temperatures. A similar result may be true for the disordered alloy problem. In the present problem it can be shown that there exists a tail in the density of states below the edge given by the retraceable-path approximation.[11] The mobility is undoubtedly nonzero for these states in the tail as well as those in the bulk of the band, so that there is no mobility edge as in the disordered system problem. However, the mobility may become exponentially small in the tail, so that the results near the edge may have qualitative validity.

In conclusion we would like to comment on the sign of the Hall effect in our calculation. We find that a Mott-Hubbard band acts like a normal band in a semiconductor in that holes give rise to a positive Hall effect and electrons to a negative Hall effect in agreement with the conclusions of Bari *et al.*[18] This point was emphasized by Geballe[19] who pointed out its importance with respect to doped semiconductors where, on the insulating side of the Mott transition, one observes a Hall effect which is p type even though the material is nominally n type. This arises because compensation of the donors introduces holes in the otherwise filled Mott-Hubbard band.

APPENDIX: CALCULATION OF 6th-ORDER AVERAGES

Let us consider first the average

$$S_1 = \operatorname{Tr}\langle H'^4 J_x J_y - H'^4 J_y J_x \rangle . \tag{A1}$$

To evaluate this we must enumerate all six step

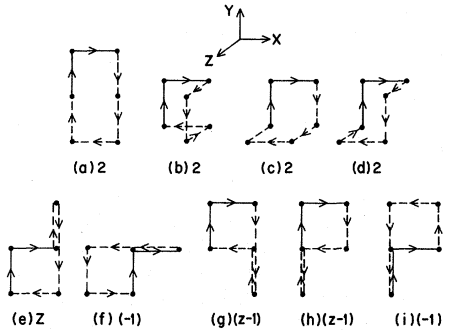

FIG. 2. Various paths which contribute to calculation of expectation value in Eq. (A1). Solid lines represent action of current operators. Dotted lines represent Hamiltonian.

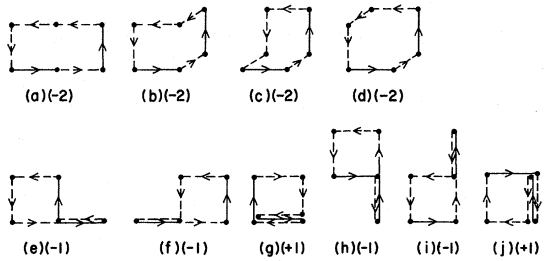

FIG. 3. Paths which contribute to calculation of expectation value in Eq. (A2). Solid lines represent action of current operators and dotted lines the Hamiltonian.

paths which involve a closed loop. In Fig. 2 we show all such paths with the first step in $+y$ direction and the second step in the $+x$ direction. The solid lines indicate which steps are taken with the J operators. In Fig. 2(a) we show a graph in which there is a single closed loop enclosing an area of $2a^2$ in the xy plane. There are two graphs of this type. In Fig. 2 below each graph we show the number of graphs of that type. In Fig. 2(f) we show a graph in which the closed loop is traversed in the anticlockwise direction. This graph will cancel the contribution linear in $\mathcal{H}$ from one of the graphs in Fig 2(e). The contribution from each graph must be weighted by the number of spins which must be ferromagnetically aligned. Thus, graphs in Figs. 2(a)–2(d) have weight $2(\frac{1}{2})^3=\frac{1}{4}$. The contributions from walks with the $J_{\pm x}$ and $J_{\pm y}$ operators will just add, and we arrive at the following value for S_1:

$$S_1 = -4e^2a^2t^6\{\tfrac{2}{16}(2i\varphi)+[\tfrac{6}{16}+\tfrac{3}{4}(z-1)](i\varphi)-\text{c.c.}\}$$
$$= -(e^3a^4t^4i\mathcal{H}/c)\,[5+6(z-1)]. \qquad \text{(A2)}$$

We also need the average

$$S_2 = \mathrm{Tr}\langle H'J_xH'^3J_y - H'J_yH'^3J_x\rangle . \qquad \text{(A3)}$$

Again let us consider first only paths with the steps by the current operators in the $+x$ and $+y$ directions. In Figs. 3(a)–3(d) we show all such paths which are a single closed loop of six steps. Path in Fig. 3(a) is confined to the xy plane and encloses an area $2a^2$ whereas the others enclose an area a^2. In Figs. 3(c)–3(j) we consider all the graphs where we retrace one of the current operator steps. Only those graphs confined to xy plane enclose an area in that plane. As before the graphs with steps with the $\pm x$ and $\pm y$ current operators add to order $\mathcal{H}^2$ and we arrive at the result

$$S_2 = -4e^2a^2t^6[\tfrac{2}{16}(-2i\varphi)+(\tfrac{6}{16}+\tfrac{2}{4})(-i\varphi)+\text{c.c.}]$$
$$= 9ie^3a^4t^6\mathcal{H}/\hbar c . \qquad \text{(A4)}$$

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