Transport coefficients in the Hubbard model with repulsion

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The anomalous temperature dependence, determined by scattering of electrons whose energy is close to a Fermi surface intersecting van Hove singularities, of the conductivity and Hall constant is calculated. © *1995 American Institute of Physics.*

The temperature dependence of the transport coefficients in a metal is determined by the electron-phonon and electron-electron part of the collision integral. In a wide temperature range, scattering of electrons by phonons makes the main contribution to the resistance. At low temperatures, however, electron-electron scattering processes play the main role. In the present paper an electronic system with strong repulsion in the same cell, which results in splitting of the allowed electron band into bottom and top subbands, is studied. In the limit of infinite Hubbard energy, it is sufficient to study only the bottom subband, which has the same electronic spectrum $\epsilon(\mathbf{p})$ as in the tight-binding approximation, but the hopping integral depends on the number of electrons (n) per unit cell:[1]

$$\xi\mathbf{p}=f\epsilon(\mathbf{p})-\mu. \tag{1}$$

Here f is the so-called end factor: $f=1-n/2$—for the bottom Hubbard subband and $f=n/2$—for the top subband.

The chemical potential μ is determined in terms of the electron density n by means of the equation of state, which in our approximation (Hubbard I) for the bottom subband has the form:

$$n=2f\,\Sigma\mathbf{p}\; n_F(\xi\mathbf{p}), \tag{2}$$

where $n_F(\epsilon)$ is the Fermi distribution function.

Cluster calculations[2] for a square lattice give in the limiting case of infinite Hubbard energy an equation of state $n=n(\mu)$ at $T=0$ which is qualitatively identical to Eq. (2).

In the present paper the characteristic features of the temperature dependence of the electron-electron collision integrals are studied under the condition that the Fermi surface passes near van Hove singularities. In the simplest cases of square and bcc lattices, zero Fermi energy and $n=2/3$ correspond to the points of the van Hove singularities.

We seek the solution of the transport equation in the standard form: $\Phi(\mathbf{p})=n_F(\xi\mathbf{p})-n_F'(\xi\mathbf{p})g(\mathbf{p})$. The equation linearized with respect to the small correction $g(\mathbf{p})$ can then be written in the form:

$$n_F'(\xi\mathbf{p})\left\{e(\mathbf{E}\cdot\mathbf{v})-\frac{e}{c}[\mathbf{v}\times\mathbf{H}]\,\frac{\partial g}{\partial\mathbf{p}}\right\}=-\hat{J}^{st}(g). \tag{3}$$

In the zeroth approximation of the magnetic field **H**, it is natural to seek the solution $g_0(\mathbf{p})$ of the transport equation in the form of products of $e(\mathbf{E}\cdot\mathbf{v})$ by an unknown function of the excitation energy $\tau_0(\xi\mathbf{p})$: $g_0(\mathbf{p})=e(\mathbf{E}\cdot\mathbf{v})\tau_0$. To a first approximation of the magnetic field directed along the z axis, we obtain the following equation for $g_1(\mathbf{p})$:

$$H\frac{e^2}{c}n_F'(\xi\mathbf{p})\left\{E_\alpha\frac{\partial v_\alpha}{\partial p_y}v_x-E_\alpha\frac{\partial v_\alpha}{\partial p_x}v_y\right\}\tau_0=-\hat{J}^{st}(g_1). \tag{4}$$

Therefore, if the entire angular dependence of the zeroth approximation is determined by the factor $(\mathbf{E}\cdot\mathbf{v})$, then in the linear approximation in the magnetic field the angular dependence is determined by the factor in braces on the left-hand side of the integral equation (4).

In the simplest case of a square lattice $\epsilon\mathbf{p}=-\cos p_x-\cos p_y$,

$$g_0=e\tau_0E_\alpha\sin p_\alpha;\quad g_1=e^2H\tau_1\tau_0(-E_x\cos p_x\sin p_y+E_y\cos p_y\sin p_x)/c. \tag{5}$$

If it is assumed that the functions τ_0 and τ_1 have no singularities, then the conductivity σ and the Hall constant R are determined by integrals over the Fermi surface:

$$\sigma=e^2\tau_0\langle(\sin p_x)^2\rangle/m^*;\ \tan\theta=E_y/E_x=e\tau_1H\langle(\sin p_y)^2\cos_x\rangle/m^*c\langle(\sin p_y)^2\rangle, \tag{6}$$

$$R=E_y/E_xH_\sigma=\tau_1\langle(\sin p_y)^2\cos p_x\rangle/c\tau_0e\langle(\sin p_y)^2\rangle\langle(\sin p_x)^2\rangle,$$

where the angular brackets indicate integration with the factor $\delta(\xi\mathbf{p})$. In what follows, it is assumed that the effective mass $m^*=1$.

The minimum value of the chemical potential corresponds to the point $P(0,0)$ near which the sign of the Hall constant coincides with the sign of the charge e. As the density increases, the quantity $|R|$ decreases to zero, and at some concentration the sign of R is different from the sign of the charge e. This corresponds to additional filling of the bottom Hubbard subband. For a square lattice all averages $\langle\ldots\rangle$ in Eq. (6) can be expressed in terms of the complete elliptic integrals of the first and second kinds $K(k)$ and $E(k)$ with the argument $k=\sqrt{1-(\mu/2f)^2}$; $\langle(\sin p_\alpha)^2\rangle=2[E(k)-(1-k^2)K(k)]/\pi^2$;

$$\langle(\sin p_\alpha)^2\cos p_\beta\rangle=-\mu[K(k)-E(k)]/2\pi^2f. \tag{7}$$

Therefore, the Hall constant vanishes at $\mu=0$ for the energy surface that passes through the van Hove singular points: $A=(0,\pi)$ and $B=(\pi,0)$.

As follows from relations (6), the conductivity and Hall constant are determined by two relaxation times, which should be sought from the solution of the transport equation.

To write the transport equation, it is necessary to know the quantum-mechanical transition probability W for scattering with prescribed momenta p_k and spins σ_k. This probability is expressed in terms of the exact scattering amplitude. It was calculated in the Born approximation by the present author in Ref. 3 . We assume that the electron density is close to the value 2/3 ($|\mu|\ll1$). If the excitation energy $\xi_p=-(\cos p_x+\cos p_y)-\mu$, then near the van Hove points $A(p_x=0,\ p_y=\pi)$ and $B(p_x=\pi,\ p_y=0)$ the excitation energies are hyperbolic and the effective masses in them have opposite signs:

$$\xi_k^a=(k_x^2-k_y^2)/2-\mu; \quad \xi_q^b=(-q_x^2+q_y^2)/2-\mu. \tag{8}$$

To find the temperature dependence of the resistivity $\rho(T)$, we employ a variational principle (see, for example, Ref. 4):

$$\rho(T)=\sum W[\psi_1+\psi_2-\psi_3-\psi_4]^2\prod_{k=1}^{4}\{\mathrm{sech}(\xi\mathbf{p}_k/2T)\}(1/8T\mathbf{D}^2). \tag{9}$$

Here the summation extends over the momenta $\mathbf{p}_{1,2}$ of the scattering particles and $\mathbf{p}_{3,4}$ of the scattered particles; W is the scattering probability; since the vector $\mathbf{D}$ is the integral of $4e\psi v$ over the Fermi surface, it must be assumed that it does not depend on the temperature.

We introduce the variables $\mathbf{q}=\mathbf{p}_3-\mathbf{p}_1=\mathbf{p}_2-\mathbf{p}_4$, $2\mathbf{p}=\mathbf{p}_1+\mathbf{p}_3$, $2\mathbf{p}'=\mathbf{p}_2+\mathbf{p}_4$, and then we employ, in the case of a two-dimensional lattice, instead of the four momentum variables $\mathbf{p}$ and $\mathbf{p}'$ the energy variables $u,u',v=-v'=\Omega$:

$$2u=\xi(p_3)+\xi(p_1); \quad 2u'=\xi(p_4)+\xi(p_2); \quad 2v=\xi(p_3)-\xi(p_1);$$

$$2v'=\xi(p_4)-\xi(p_2),$$

where $\xi(p)$ is the excitation energy (1). Separating the integrals over the transferred energy Ω and the transferred momentum q, we obtain

$$\rho(T)=\int \frac{dudu'd\Omega W[\psi_1+\psi_2-\psi_3-\psi_4]^2\Pi_\Omega(u)\Pi_\Omega(u')d\mathbf{q}}{Jk_{\mathbf{q}}(\Omega,u)Jk_{-\mathbf{q}}(-\Omega,u')\sinh^2(\Omega/T)8T\mathbf{D}^2}. \tag{10}$$

Here $\Pi_\Omega(u)=\tanh[(u+\Omega)/2T-\tanh[(u-\Omega)/2T]$, $Jk_q(\Omega,u)$ is the Jacobian of the transformation from the variables u,u',Ω to the variables p,p' with fixed q. In the limiting case of low temperatures the quantity $\Pi_\Omega(u)$ is of a step character: $\Pi_\Omega(u)+2\mathrm{sign}\Omega\{\theta(\Omega^2-u^2)\}$, so that the region of integration over the variables u,u', and Ω is of order T^3. If the Fermi surface passes near van Hove points, $|\mu|\ll 1$, the Jacobians are of the order of the largest of $-T$ or $|\mu|$. We thus conclude that in the region of the lowest temperatures $T\ll|\mu|\ll 1$ the Jacobians are of the order of $T^2/|\mu|$, so that the resistance increases as $T^2/|\mu|$. In the region of the high temperatures $1\gg T\gg|\mu|$ the Jacobians are of order T and for this reason the resistance increases linearly (since $\int d\mathbf{q}\approx T$).

The estimates presented above are valid under the natural assumption that the symmetrized combination of the trial functions $\psi_1+\psi_2-\psi_3-\psi_4$ does not vanish and has no singularities in the important region of integration over both the energy variables and the transferred momentum variables q. To analyze the possible variants, we choose a trial function equal to the velocity in one of the principal directions (α) $\psi=\sin\alpha$ and we study four types of collision integrals corresponding to scattering by different van Hove points. a) In the case of scattering between identical points $A_1+A_2+A_3+A_4$ the linear combination of the trial functions $G=\sin\alpha_1+\sin\alpha_2-\sin\alpha_3-\sin\alpha_4$, expressed in terms of the momentum transfer $\mathbf{q}$ and the momenta $\mathbf{p}=(\mathbf{p}_3+\mathbf{p}_1)/2$, $\mathbf{p}'=(\mathbf{p}_4+\mathbf{p}_2)/2$ in a given direction α, has the form:

$$G=2\sin(q/2)[\cos p'-\cos p]. \tag{11}$$

b) For scattering with umklapp $A_1+A_2\to B_3+B_4$ the momenta $\alpha_{3,4}=\pi+p_{3,4}$ and $\alpha_{1,2}=p_{1,2}$, but we have, as before, $\mathbf{p}=(\mathbf{p}_3+\mathbf{p}_1)/2$, $\mathbf{p}'=(\mathbf{p}_4+\mathbf{p}_2)/2$, so that

$$G=2\cos(q/2)[\sin p'+\sin p]. \tag{12}$$

c) In the case of scattering by different van Hove points $A_1+B_2\to A_3+B_4$, when $\alpha_{1,3}=p_{1,3}$ and $\alpha_{2,4}=\pi+p_{2,4}$, we have

$$G=-2\sin(q/2)[\cos p'+\cos p]. \tag{13}$$

d) In the case of scattering with a large momentum transfer, close to half the reciprocal lattice vector $A_1+B_2\to B_3+A_4$, when $\alpha_{1,4}=p_{1,4}$ and $\alpha_{2,3}=\pi+p_{2,3}$, we have

$$G=2\cos(q/2)[\sin p-\sin p']. \tag{14}$$

We note that for the hyperbolic model (p, $p'\to 0$) in case a) the trial function G vanishes. This corresponds in an obvious way to vanishing of the contribution from normal scattering processes. In this limit the largest contribution comes from case c) — scattering of particles with effective mass of opposite sign and low momentum transfer — Baber scattering.[5]

The scattering with umklapp — case b) and also case d) in the hyperbolic model (8) make a contribution of the order of the square of the momenta p or p', which ultimately leads to the appearance of an extra factor of T compared to case c).

In the low-temperature limit the power-law contribution, acccording to Eq. (10), comes from a region of low transferred energy $\Omega\leqslant T$. In the limit $\Omega\to 0$ with a fixed momentum transfer q the regions of integration over the momenta p and p' are identical in cases a) and d), while in case b) their signs are different. It can be concluded, therefore, that the case $A_1+B_2\to A_3+B_4$ makes the main contribution. If it is assumed that the probability of this scattering process does not vanish and has no singularities on the van Hove energy surface, then the linear behavior of the resistance starts at temperatures of the order of $|\mu|$. At low temperatures $T\ll|\mu|$ we obtain the same dependence T^2 as in the Landau–Pomeranchuk theory,[6] but enhanced by the factor $\ln(|\mu|/T)$.

To calculate the temperature dependence of the orbital relaxation time τ_1, we employ again a variational principle. According to Eq. (6), in the τ-approximation the Hall constant R can be expressed in terms of the ratio of the reciprocal $1/\tau_0$ of the longitudinal relaxation time and the reciprocal $1/\tau_1$ of the transverse relaxation time. In general, the entire temperature dependence is determined by the ratio of the integrals:

$$R/R_0\cong\{[\psi_1+\psi_2-\psi_3-\psi_4]\}^2/\{[\varphi_1+\varphi_2-\varphi_3-\varphi_4]^2\}, \tag{15}$$

where the braces indicate integration over all energy and angular variables with the same factors as in Eq. (10). Here φ_k is a trial function, which corresponds to the left side of the transport equation (4), which is linearized with respect to the external magnetic field. If the velocity in the principal direction α is chosen as the trial function ψ, then the function φ must be sought in the form $\sin\alpha\ \cos\beta$, where β is the dimensionless momentum in a different principal direction. At a transition from one van Hove point to another, the function φ does not change. For this reason, the linear combination $F=\varphi_1+\varphi_2-\varphi_3-\varphi_4$ has the same form for all four singular collision integrals (11)–(14), i.e. for cases a, b, c, and d:

$$F=-2\{c_y\ s_x\cos(p_x)\cos(p_y)-s_yc_x\sin(p_x)\sin(p_y)\}+2\{p_x\to p'_x;p_y\to p'_y\}. \qquad (16)$$

Here $s_\nu=\sin(q_\nu/2)$, $c_\nu=\cos(q_\nu/2)$, and $\nu=x,y$. We see that in the hyperbolic limit the trial function F depends on the products of momenta $p_\lambda p_\nu$ or $p'_\lambda p'_\nu$. Moreover, it vanishes when the momenta p and p' are equal, when the momenta p and p' have different signs, and also when the momenta p and p' differ by half a reciprocal lattice vector $p-p'=(\pi,\pi)$. There properties of the function F lead to the fact that the integration over the energy variables u and u' with the function F^2 in the limit $T\ll 1$ gives a factor Ω^4, while after integrating with the function $\mathbf{G}=\mathbf{v}_1+\mathbf{v}_2-\mathbf{v}_3-\mathbf{v}_4$ the leading term is of order Ω^2. The integration of power-law functions with the factor $\sinh^{-2}(\Omega/T)$ determines the temperature dependence of expression (15).

The temperature dependence of the Hall constant thus appears because the temperature dependence of the transverse relaxation time is different from that of the longitudinal relaxation time. The temperature expansion of the inverse transverse relaxation time starts with the power T^4 at low temperature and the power T^3 at high temperature. The expansion of the reciprocal of the longitudinal relaxation time starts with the power T^2 at low temperatures and T at high temperatures, but it contains anisotropic terms of the same order of magnitude as in the case of the reciprocal of the transverse relaxation time. We therefore conclude that for electronic densities at which the Fermi surface is close to van Hove singularities the Hall constant increases with decreasing temperature

$$R\cong A+(B/T)+(C/T^2). \qquad (17)$$

The coefficients A, B, and C depend strongly on the position of the Fermi level. All three coefficients change sign when the van Hove singularities lie on the Fermi surface.

The existence of a temperature range where the resistance is a linear function of the temperature is also determined by the closeness to van Hove singularities. At temperatures lower than the energy distance from the van Hove surface the temperature dependence of the resistance is quadratic.

All three phenomena are characteristic of the two-dimensional Hubbard model and are manifested when the scattering probability (W) on the Fermi surface does not vanish and has no singularities. Calculations of the scattering amplitude, in terms of which the scattering probability W is expressed, can be made on the basis of the parquette approximation.[7] This is a subject which will be considered separately.

As follows from the general expression (16), the qualitative form of the temperature dependence of the Hall constant (17) remains unchanged if the transition probability is a power-law function of the energy transfer Ω. As far as the temperature dependence of the resistivity is concerned, there are two possibilities. 1) The above-considered case in which the transition probability is finite in a wide energy range near the Fermi surface. In this case the resistance has a linear temperature dependence in the temperature range starting with some characteristic temperature T_0, which depends on the closeness of the electron density n to the value n_0 for which the Hall constant vanishes. If $T\leqslant T_0$, then the resistance increases according to a law close to T^2. For $n=n_0$ we have a linear law at all temperatures. Laws of this type are observed in experiments on $Ln_{2-x}Sr_xCuO_4$ (Ref. 8). According to our interpretation, the temperature T_0 implies that the Fermi surface is close to the energy surface that experiences van Hove singularities. The case 2)

corresponds to the case in which the scattering amplitude vanishes on the van Hove surface. This is obtained in the Born approximation for the classical Hubbard model.[2] In this situation the scattering from singular points is no more important than the scattering from the rest of the Fermi surface. For this reason, the quadratic law for the resistance applies in a wide temperature range, as is the case in $Nd_{2-x}Ce_xCuO_4$ (Ref. 9). In the compound $YBa_2Cu_3O_{7-\delta}$ an anomalous temperature dependence of the Hall constant was observed in Ref. 10, in agreement with Eq. (17).

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