Reactive Hall constant of Strongly Correlated Electrons

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The zero-temperature Hall response within tight-binding models of correlated electrons is studied. Using the linear response theory and a linearization in the magnetic field \( B \), a general relation for the reactive (zero frequency) Hall constant \( R_H^0 \) in the fast (transport) limit is derived, involving only matrix elements between the lowest excited states at \( B = 0 \); for noninteracting fermions, the Boltzmann expression is reproduced. For a Fermi liquid with a well defined Fermi surface and linear gapless excitations an analogous expression is found more generally. In the specific case of quasi-one-dimensional correlated systems a relation of \( R_H^0 \) to the charge stiffness \( D \) is recovered. Similar analysis is performed and discussed for \( D \) and the compressibility.

I. INTRODUCTION

Properties of metals with strongly correlated electrons can be strikingly inconsistent with the usual picture of ordinary Fermi liquid. The most intensively studied example are the superconducting cuprates \(^1\), which behave in the normal state as hole doped magnetic (or Mott-Hubbard) insulators. Here an evident and challenging problem is to reconcile the Hall constant \( R_H^0 \), following approximately a simple semiclassical behavior \( R_H^0 \sim 1/n_{\text{h}}e_0 \) consistent with an (semiconductor-like) interpretation of low concentration \( n_{\text{h}} \) of holes in an insulator, with the evidence for large Fermi surface as it emerges e.g. from photoemission experiments.

The theoretical analysis of the Hall constant \( R_H^0 \) and more generally of the dynamical Hall response \( R_H(\omega) \) in systems with correlated electrons has proved to be very difficult. Within the general linear response theory the procedure for the calculation of Hall response is in principle well established \(^2\) and requires the introduction of a modulated magnetic field \( B \exp(iq\mathbf{r}) \) and consequently a modulated vector potential \( \mathbf{A} \) in order to formally allow a linearization of the offdiagonal conductivity \( \sigma_{\beta\alpha} \) in \( B \neq 0 \) and to derive an expression for \( R_H(q, \omega) \) not involving \( B \).

At \( T = 0 \) the relevant case for usual transport measurements of d.c. \( R_H^0 \) is the limit: \( q \to 0 \) first, and then \( \omega \to 0 \) \(^3\). The formulation originally designed for nearly free electrons has been extended to tight-binding models for strongly correlated electrons \(^4\). Nevertheless there have been so far rather few results for strongly correlated models obtained following this framework. The Hall mobility of a single carrier at large \( T \) has been evaluated \(^5\). \( R_H(\omega) \) has been calculated in the high-\( \omega, T \) expansion \(^6\), indicating on the change of sign of \( R_H \) in the vicinity of the Mott-Hubbard insulator. One of the present authors \(^7\) also showed a plausible but nontrivial result that a single carrier doped into a magnetic insulator at \( T = 0 \) indeed follows the semiclassical formula for \( R_H^0 \).

More direct numerical evaluation of \( R_H^0 \) within the linear response approach (at finite \( B > 0 \)) is also quite delicate for prototype models of correlated electrons. Namely, small-system studies give even some controversial conclusions regarding the sign of \( R_H^0 \) close to the magnetic insulator \(^8\). \(^9\) It has been shown \(^10\) that a better controlled approach at \( T = 0 \) can be obtained for a system with open boundary conditions in one direction, i.e. on a ladder geometry, where \( R_H^0 \) can be expressed in terms of derivatives of the ground state energy with respect to external fields.

Recently, the present authors \(^11\) derived at \( T = 0 \) a quite general relation between the reactive Hall constant \( R_H^0 \) and the derivative of the charge stiffness \( D \) with respect to the electron density \( n \),

\[
R_H^0 = -\frac{1}{e_0 D} \frac{\partial D}{\partial n} .
\]

It should be pointed out that the derivation uses, in the direction transverse to the driving field, the non-standard (slow) limit \( \omega \to 0 \) first, then \( q \to 0 \). It is a question and also our aim to find out whether or under which conditions this relation applies to the more relevant fast limit: \( q \to 0 \), then \( \omega \to 0 \). Eq.\(^1\) has some very attractive properties for the analysis of strongly correlated electrons: a) \( D \) is at \( T = 0 \) the central quantity distinguishing the Mott-Hubbard insulator from a conductor (metal), b) close to the Mott-Hubbard insulator where the stiffness is expected to be proportional to hole doping, i.e. \( D \propto n_{\text{h}} = 1 - n \), Eq.\(^1\) directly implies the plausible semiclassical result \( R_H^0 = 1/e_0 n_{\text{h}} \), which has been hard to establish by any other analytical method so
far.

A qualitatively similar relation to Eq. (1) was also proposed in Ref. [3], where \( \sigma_{xy} \) was related to the variation of the kinetic energy, i.e., \( \partial (T)/\partial n \). Note that in a tight binding system \( (T) \) and \( D \) are interrelated through the optical sum rule.

Our goal is to express the \( T = 0 \) reactive Hall constant \( R^0_H \) in terms of eigenstates of correlated electrons in the absence of \( B \) and the fast limit, \( q \to 0 \) first and then \( \omega \to 0 \). The present approach is the extention of the previous analysis for a single carrier to the general electron concentration \( n \). As first formulated by Kohn [13], the diagonal conductivity in a metal is singular (reactive) at \( \omega = 0 \), and a more specific one for Fermi liquids with a Fermi liquid, and in particular the quasi-1D system where analysis we discuss noninteracting fermions, an isotropic relaxation-time approximation. As the application of the new formulation to Eq.(1) as well as to the \( T = 0 \) limit, obtaining an expression analogous to the one in the standard Boltzmann theory for a single relaxation-time approximation [15, 16].

The paper is organized as follows: In Sec. II we introduce the linear response formalism for \( R^0_H \) in metals within the single relaxation-time approximation [14, 15].

The dynamic Hall response is given by

\[
R_H(\omega) = \frac{\varepsilon^x_y(\omega)}{B|J_x(\omega)|} = \frac{1}{B \sigma_{xx}(\omega) \sigma_{yy}(\omega)} \left| \frac{\partial}{\partial \omega} \right|_{\omega \to 0, q \to 0} ,
\]

where \( \sigma_{\alpha\beta} \) denote the conductivities at \( B \neq 0 \) and at \( B = 0 \), respectively, higher order terms in \( B \) have already been neglected in Eq. (1); the hat will denote quantities in magnetic field from here on and we are interested in the limit \( q \to 0, B \to 0 \).

Models for strongly correlated electrons are usually analyzed within the tight binding framework \( H = T + H_{int} \) where the magnetic field (flux) enters through the kinetic energy \( T \) via the Peierls phase, i.e.

\[
T = - \sum_{(ij)s} t_{ij} [e^{i(\theta_{ij} + \phi_{ij})} c^\dagger_{js} c_{is} + H.c.] ,
\]

Here it is meaningful to distinguish the phase due to a constant magnetic field \( B \) (which in principle can be large), i.e. \( \theta_{ij} = e r_{ij} \cdot A(r = R_{ij}) \), and the small driving (time dependent field) \( \phi_{ij}(t) = e r_{ij} \cdot \phi(r = R_{ij}) \) where \( r_{ij} = r_j - r_i \) and \( R_{ij} = (r_i + r_j)/2 \); the sum \( (ij) \) runs over pairs of sites. The (particle) current \( J \) can be defined as,

\[
J^p_\alpha = - \frac{1}{e} \frac{\partial T}{\partial \phi^\alpha} = \hat{J}^p_\alpha - e \hat{\tau}^p_\alpha \sigma^0_{\alpha\beta} ,
\]

where \( \hat{J}^p_\alpha \) and \( \hat{\tau}^p_\alpha \) refer to the paramagnetic current and stress tensor (diamagnetic contribution), respectively, both in the presence of finite \( A \),

\[
\hat{J}^p_\alpha = \sum_{(ij)s} t_{ij} r_{ij} c^\dagger_{js} e^{i p \cdot R_{ij}} (e^{i \theta_{ij}} c_{is} + H.c.) ,
\]

\[
\hat{\tau}^p_{\alpha\beta} = \sum_{(ij)s} t_{ij} r_{ij} c^\dagger_{js} e^{i p \cdot R_{ij}} (e^{i \theta_{ij}} c_{is} + H.c.) .
\]

The conductivity tensor at \( B \neq 0 \), as a linear response to \( \phi^\alpha_\beta(t) \), can be expressed as [15, 16],

\[
\tilde{\sigma}_{\alpha\beta}(\omega) = \frac{i e^2}{N \omega} \left\{ \tilde{\chi}_{\alpha\beta}(\omega) \right\} ,
\]

\[
\tilde{\chi}_{\alpha\beta}(\omega) = i \int_0^\infty dt e^{i \omega t} \langle \tilde{J}^0_\beta(t), \tilde{J}^0_\alpha \rangle B ,
\]

where \( N \) is the number of cells (volume of the unit cell is assumed unity) and \( \langle \cdot \rangle_B \) denote averages at \( B \neq 0 \).
A. Linearization in B

In order to calculate \( R_H(\omega) \) we have to evaluate \( \hat{\sigma}_{yx} \) up to the linear term in \( B \). Since \( \langle \hat{\tau}^{q_y} \rangle = 0 \), we need

\[
\hat{\chi}_{yx}(\omega) = -eA^qK_{yx}(\omega) .
\]  

(9)

In a conductor at \( T = 0 \) the conductivities \( \sigma_{\alpha\alpha}^0 \) are singular at \( \omega = 0 \) [3] defining the charge stiffness \( D_{\alpha\alpha}^0 \),

\[
\sigma_{\alpha\alpha}^0(\omega) = \frac{2ie^2}{\omega}D_{\alpha\alpha}^0 + \sigma_{\alpha\alpha}^{reg}(\omega) ,
\]

(10)

where \( \sigma_{\alpha\alpha}^{reg}(\omega) \) is the regular part of the conductivity. In the same limit \( K_{xy}(\omega) \) is also expected to be singular leading to a finite \( R_H^0 = R_H(\omega \to 0) \). Hence we define the off-diagonal stiffness

\[
\Lambda_{yx} = \left[ \frac{\omega K_{yx}(\omega)}{4Nq} \right]_{\omega \to 0} ,
\]

(11)

so that we can express the reactive Hall constant as

\[
R_H^0 = \frac{\Lambda_{yx}}{eD_{yx}^0D_{yy}^0} .
\]

(12)

Performing now the linearization in the static vector potential \( A^q \) we take into account the analogy to Eq. (10) and the coupling to the field,

\[
\hat{j}_o^p = j_o^p - \tau_{\alpha\alpha}^{p-x-q}A^q , \quad \hat{H}' = -\hat{e}_x^q A^q ,
\]

(13)

where \( j_o^p = j_o^p(B = 0) \) and \( \tau_{\alpha\alpha}^{p-x-q} = \tau_{\alpha\beta}^{p}(B = 0) \). Instead of a general formalism at \( T > 0 \) [3] we assume here explicitly \( T = 0 \) and we can express

\[
\hat{\chi}_{yx} = \langle 0_B | j_y^q \frac{1}{\omega + \hat{E}_0 - \hat{H}} j_x^q | 0_B \rangle

- \langle 0_B | \frac{1}{\omega + \hat{E}_0 + \hat{H}} j_y^q | 0_B \rangle = \chi^I_{yx} + \chi^{II}_{yx} ,
\]

(14)

where \( | 0_B \rangle , \hat{E}_0 , \hat{H} \) refer to \( B \neq 0 \). We consider only linear terms in \( A^q \) therefore \( \hat{E}_0 = 0 \). Taking into account that

\[
| 0_B \rangle \sim | 0 \rangle - eA^q \frac{1}{E_0 - \hat{H}} j_x^q | 0 \rangle ,
\]

\[
\frac{1}{X - Y} \sim \frac{1}{X} + \frac{1}{X} \frac{1}{Y} ,
\]

(15)

we obtain

\[
K_{yx}^{I} = \langle 0 | j_y^q \omega - (H - E_0) j_x^q | 0 \rangle

+ \langle 0 | \frac{1}{\omega - (H - E_0)} j_x^q | 0 \rangle

+ \langle 0 | j_y^q \omega - (H - E_0) j_x^q | 0 \rangle

+ \langle 0 | \frac{1}{E_0 - \hat{H}} j_y^q \omega - (H - E_0) j_x^q | 0 \rangle

+ \langle 0 | j_y^q \omega - (H - E_0) j_x^q \omega - (H - E_0) j_x^q | 0 \rangle ,
\]

(16)

with an analogous expression holding for \( K_{yx}^{II} \).

B. Fast limit

It is helpful to express \( K_{yx}(\omega) \) in terms of eigenstates. Assuming that the ground state \( | 0 \rangle \) has momentum \( \mathbf{Q} \) it is convenient to separate excited states into sectors: \( | m \rangle \) with momentum \( \mathbf{Q} , | \tilde{m} \rangle \) with \( \mathbf{Q} - \mathbf{q} \), and \( | \overline{m} \rangle \) with \( \mathbf{Q} + \mathbf{q} \). Denoting \( \epsilon = E - E_0 \) and using

\[
\frac{1}{(\omega - \epsilon_{\tilde{m}})(\omega - \epsilon_l)} = \frac{1}{\epsilon_{\tilde{m}} - \epsilon_l} \left( \frac{1}{\omega - \epsilon_{\tilde{m}}} - \frac{1}{\omega - \epsilon_l} \right) ,
\]

(17)

we can write

\[
K_{yx}(\omega) = \sum_{m} \left[ \frac{\gamma_{\tilde{m}}}{\omega - \epsilon_{\tilde{m}}} + \frac{\gamma_l}{\omega + \epsilon_l} \right]

+ \sum_{m>0} \left[ \frac{\delta_m}{\omega - \epsilon_m} + \frac{\delta_l}{\omega + \epsilon_m} \right] ,
\]

(18)

where

\[
\gamma_{\tilde{m}} = 2(j_y^q)_{\tilde{m}}(d_{xx}^q)_{\tilde{m}0} ,
\]

\[
2(d_{xx}^q)_{\tilde{m}0} = (\tau_{xx}^q)_{\tilde{m}0} - \sum_{l>0} \frac{(j_y^q)_{\tilde{m}l}(j_x^q)_{l0}}{\epsilon_l - \epsilon_m}

- \sum_{l} \frac{(j_x^q)_{l\tilde{m}}(j_y^q)_{l0}}{\epsilon_l} ,
\]

(19)

and

\[
\delta_m = 2(d_{yx}^0)_{m0}(j_x^q)_{m0} ,
\]

\[
2(d_{yx}^0)_{m0} = (\tau_{yx}^q)_{m0} - \sum_{l} \frac{(j_y^q)_{ql}(j_x^q)_{lm}}{\epsilon_l - \epsilon_m}

- \sum_{l} \frac{(j_x^q)_{ql}(j_y^q)_{lm}}{\epsilon_l} ,
\]

(20)

and analogous expressions for \( \tilde{\gamma}_{\tilde{m}} \) and \( \tilde{\delta}_m \). Since we are interested in the limit \( q \to 0 \) it follows anyway from \( \sigma_{\alpha\beta}(\omega) = \sigma_{\alpha\beta}(\omega) \) that \( \tilde{\gamma}_{\tilde{m}} = \gamma_{\tilde{m}} \) = real and \( \tilde{\delta}_m = \delta_m \) = real.

The fast limit corresponds taking first \( q \to 0 \) and then \( \omega \to 0 \). In Eq. (18) the singular part \( \propto 1/\omega \) in this case emerges from the class of excited states \( \mathcal{M} \) which exhibit \( \epsilon_m \to 0 \) in the \( q \to 0 \) limit. On the other hand \( \delta_m , \tilde{\delta}_m \) terms are not contributing since \( \epsilon_m > 0 \) do not depend on \( q \) and remain finite in the limit \( q \to 0 \). \( \Lambda_{yx} \) can therefore be expressed as

\[
\Lambda_{yx} = \lim_{q \to 0} \frac{1}{2Nq} \sum_{\tilde{m} \in \mathcal{M}} \gamma_{\tilde{m}} = \lim_{q \to 0} \frac{1}{Nq} \sum_{\tilde{m} \in \mathcal{M}} (j_y^q)_{\tilde{m}0}(d_{xx}^q)_{\tilde{m}0} .
\]

(21)

We note that \( (d_{xx}^q)_{\tilde{m}0} \) can also be represented as the
matrix element of the stiffness operator $d_{\alpha\alpha}^{-q}$,
\[
(d_{\alpha\alpha}^{-q})_{\hat{m}\hat{n}} = \langle \hat{m} | d_{\alpha\alpha}^{-q} | \hat{n} \rangle = \frac{1}{l} \langle \hat{m} | j_{\alpha\alpha}^{-q} \rangle
\]
\[
- j_{\alpha\alpha}^{-q} \frac{1}{H - E_{\hat{m}}} j_{\alpha\alpha}^{0} - j_{\alpha\alpha}^{0} \frac{1}{H - E_{\hat{n}}} j_{\alpha\alpha}^{-q} | \hat{n} \rangle ,
\]
provided that $(\rho_{\alpha})_{\hat{m}\hat{n}} = 0$. It is quite evident that the operator $d_{\alpha\alpha}^{-q}$ is closely related to the charge stiffness since it follows from Eq. (10) that $D_{\alpha\alpha}^{0} = (\rho_{\alpha})_{\hat{m}\hat{n}}/N$.

Moreover, there are other more compact representations of $(d_{xx}^{-q})_{\hat{m}\hat{n}}$. We first note that it just the matrix element at $B > 0$,
\[
(d_{xx}^{-q})_{\hat{m}\hat{n}} = \frac{i q}{2} \frac{\partial}{\partial B} (m_{B} j_{xx}^{0} | 0_B \rangle ,
\]
as follows directly from Eq.(14) by using the representation of $| m_{B} \rangle$ states and extracting the singular term at $q \to 0$,
\[
\chi_{\mu\nu} = \sum_{m_{B}} \langle 0_B | j_{\mu}^{q} m_{B} \rangle \frac{1}{\omega + E_{0} - E_{m}} \langle m_{B} | j_{\nu}^{0} | 0_B \rangle
\]
\[
\times \frac{1}{\omega} \sum_{\hat{m} \in \hat{M}} \langle 0 | j_{\mu}^{q} \hat{m} \rangle \langle m_{B} | j_{\nu}^{0} | 0_B \rangle .
\]

III. CHARGE STIFFNESS AND COMPRRESSIBILITY

Before proceeding with the approximations to $\Lambda_{xy}$, let us stress that also other quantities like the charge stiffness and the compressibility can be expressed solely in terms of the same excited states $\hat{m} \in \hat{M}$.

We first consider $\sigma_{\alpha\alpha}$ for $B = 0$. $D_{\alpha\alpha}^{0}$ can be expressed as
\[
D_{\alpha\alpha}^{0} = \frac{1}{N} \left[ \langle \rho_{\alpha}^{0} \rangle - \sum_{m > 0} \frac{|(\rho_{\alpha}^{0})_{mb}|^2}{\epsilon_m} \right] = \frac{1}{N} \partial^2 E_{0}(\theta_{\alpha}) ,
\]
hence $D_{\alpha\alpha}^{0}$ is evaluated from the ground state energy $E_{0}(\theta_{\alpha})$, which is the usual procedure.

Alternatively we can consider $\sigma_{\alpha\alpha}^{q}$ as the limit $q \to 0$ of $\sigma_{\alpha\alpha}^{q}$ (direction of $q$ here is arbitrary),
\[
\sigma_{\alpha\alpha}^{q}(\omega) = \frac{ie^2}{N \omega} (\langle \rho_{\alpha}^{0} \rangle - \chi_{\alpha\alpha}^{q}(\omega)) ;
\]
\[
\chi_{\alpha\alpha}^{q}(\omega) = i \int_{0}^{\infty} \frac{d \epsilon}{\epsilon} \langle \rho^{0}_{\alpha}(t) | j_{\alpha\alpha}^{-q} \rangle .
\]

In the case of $q \neq 0$ it follows $\langle \rho_{\alpha}^{0} \rangle = \chi_{\alpha\alpha}^{q}(0)$ (optical sum rule), so there is no (strictly) reactive term which would correspond to the singularity in Eq.(10). As in Sec. II we can then represent $\sigma_{\alpha\alpha}^{q}$ in terms of eigenstates,
\[
\sigma_{\alpha\alpha}^{q}(\omega) = \frac{ie^2}{N} \sum_{\hat{m} \in \hat{M}} \frac{|(\rho_{\alpha}^{0})_{\hat{m}\hat{n}}|^2}{\epsilon_{\hat{m}}} \left[ \frac{1}{\omega - \epsilon_{\hat{m}}} + \frac{1}{\omega + \epsilon_{\hat{m}}} \right] .
\]

We can nevertheless extract the reactive part as the singular part which behaves as $1/\omega$ for $q \to 0$. This again emerges from states $\hat{m} \in \hat{M}$ and consistent with Eq.(10) we get
\[
D_{\alpha\alpha}^{q} = \lim_{q \to 0} \frac{1}{N} \sum_{\hat{m} \in \hat{M}} \frac{|(\rho_{\alpha}^{q})_{\hat{m}\hat{n}}|^2}{\epsilon_{\hat{m}}} .
\]

Eqs. (27) and (30) define two alternative approaches to evaluate $D_{\alpha\alpha}^{q}$, where the first is the standard one. The equivalence of both is expected to give more insight into the excited states and matrix elements $(\rho_{\alpha}^{q})_{\hat{m}\hat{n}}$. On the other hand we note that $D_{\alpha\alpha}^{q}$, Eq. (31), contains the same matrix elements as $\Lambda_{xy}$ indicating that both quantities as well as $R_{H}^{0}$ are related.

Closely related is also the generalized compressibility $\kappa^{q}$. Let us consider a perturbation induced by the modulated chemical potential so that we deal with a hamiltonian $H^{\mu} = H + \mu_{\alpha}^{q} \rho_{\alpha}^{q}$. Then we can express in analogy to $D_{\alpha\alpha}^{q}$,
\[
\kappa^{q} = \frac{1}{N} \frac{\partial \langle \rho_{\alpha}^{q} \rangle}{\partial \mu_{\alpha}^{q}} = \frac{2}{N} \sum_{\hat{m} \in \hat{M}} \frac{|(\rho_{\alpha}^{q})_{\hat{m}\hat{n}}|^2}{\epsilon_{\hat{m}}} .
\]

We also note the relation following from the conservation law for $q \to 0$,
\[
\hat{q} [H, \rho_{\alpha}^{q}] + i \epsilon \cdot j_{\alpha}^{q} = 0
\]
\[
\rightarrow q \cdot (j_{\alpha}^{q})_{I\hat{m}} = (\epsilon_{\hat{m}} - \epsilon_{I}) (\rho_{\alpha}^{q})_{I\hat{m}} ,
\]
so \((\mathbf{q})_{\ell\ell'}\) and \((\rho^q)_{\ell\ell'}\) are evidently related. From Eq.\((12)\) it follows that \((\rho^q)_{\ell\ell'} \propto q\) for \(\ell \neq \ell'\), so only states \(\ell \in \mathcal{M}\) contribute in the limit \(q \to 0\),

\[
\kappa^0 = \lim_{q \to 0} \kappa^q = \lim_{q \to 0} \frac{2}{N} \sum_{\ell \in \mathcal{M}} \frac{|(\rho^q)_{\ell\ell'}|^2}{\epsilon_{\ell\ell'}}. \tag{33}
\]

In order to find a closer relation between \(\Lambda_{yx}\) and the stiffness \(D_{\alpha\alpha}\) as e.g. manifested in Eq.\((1)\) let us consider now the stiffness \(D_{xx}^q\) in a perturbed ground state \[\mathbf{q}\].

\[
2D_{xx}^q = \frac{1}{N} \langle 0| \left[ \epsilon_{xx}^q - J_{xx}^0 \frac{1}{\epsilon_{xx}^q} \right] 0 \rangle + \frac{1}{N} \sum_{\ell \in \mathcal{M}} \left| (\rho^q)_{\ell\ell'} \right|^2 \epsilon_{\ell\ell'}, \tag{34}
\]

We can again evaluate Eq.\((34)\) within the first order of the perturbation theory in \(H' = \mu^q \rho^q\)

\[
|0_{\mu'}\rangle = |0\rangle + \sum_{\ell \in \mathcal{M}} |\ell\rangle (\rho^q)_{\ell\ell'} \frac{\mu^q}{\epsilon_{\ell\ell'}}, \tag{35}
\]

and recognize the correspondence with \(\delta_{yx}\) as explicitly expressed in Eqs.\((8),(9),(17)\) - \(20\). In fact it has been already shown \[\mathbf{q}\] that

\[
\frac{\partial D_{xx}^q}{\partial \mu^q} = \frac{q^2}{\epsilon^2 B} \delta_{yx}(0), \tag{36}
\]

Using Eqs.\((8),(18)\) and decomposing \(1/|\omega(\omega - \epsilon_m)|\) as in Eq.\((17)\), we can rewrite

\[
\delta_{yx}(\omega) = \frac{e^3 V}{qN} \left[ \sum_{\ell \in \mathcal{M}} \frac{1}{\epsilon_{\ell\ell'}} \left[ \frac{\gamma_{\ell\ell'}}{\omega - \epsilon_m} + \frac{\tilde{\gamma}_{\ell\ell'}}{\omega + \epsilon_m} \right] + \sum_{m > 0} \frac{1}{\epsilon_{m}} \left[ \frac{\delta_{m}}{\omega - \epsilon_m} + \frac{\tilde{\delta}_{m}}{\omega + \epsilon_m} \right] \right], \tag{37}
\]

taking into account that at \(q > 0\) there is no singularity strictly at \(\omega = 0\), hence terms \(1/\omega\) should cancel. For \(\omega = 0\) we get

\[
\delta_{yx}(0) = \frac{2e^3 V}{qN} \left[ \sum_{\ell \in \mathcal{M}} \frac{\gamma_{\ell\ell'}}{2\epsilon_{\ell\ell'}} + \sum_{m > 0} \frac{\delta_{m}}{2\epsilon_{m}} \right]. \tag{38}
\]

It seems plausible that in the limit \(q \to 0\) in Eq.\((38)\) only states with \(\epsilon_{\ell\ell'} \propto q\) contribute, i.e. \(\ell \in \mathcal{M}\), so that

\[
\frac{\partial D_{xx}^q}{\partial \mu^q} = \frac{2q}{N} \sum_{\ell \in \mathcal{M}} \frac{\gamma_{\ell\ell'}}{2\epsilon_{\ell\ell'}}. \tag{39}
\]

The relation to \(\Lambda_{yx}\) in Eq.\((24)\) is evident and will be exploited later on.

IV. SPECIFIC CASES

A. Single charge carrier

A nontrivial example of the above formalism is a single charge carrier i.e. a hole or an electron doped into a Mott-Hubbard insulator \[\mathbf{q}\]. We have to assume only that the carrier behaves as a quasiparticle. I.e., excited states have a well defined effective mass,

\[
\epsilon_{\ell\ell'} = ND_{yy}^0 q^2. \tag{40}
\]

For a nondegenerate ground state \(|0\rangle\) there is only one relevant excited state \(|\ell\rangle = |0\rangle\). So it follows from Eqs.\((31),(18),(24)\) that

\[
D_{yy}^0 = \frac{\langle j_y^q \rangle^2}{N\epsilon_0} \quad \rightarrow \quad |\langle j_y^q \rangle_0| = ND_{yy}^0 q , \tag{41}
\]

and

\[
\Lambda_{yx} = \frac{1}{Nq} \langle j_y^q \rangle_0 (d_{xx}^q)_{00} = \pm D_{yy}^0 D_{xx}^0. \tag{42}
\]

The semiclassical result follows finally from Eq.\((14)\),

\[
R_H^0 = \pm \frac{N}{\epsilon_0}, \quad \text{sgn}(R_H^0) = - \text{sgn}(j_y^q)_0 , \tag{43}
\]

by inserting \(e \to -e_0\). There remains to determine the sign of \(R_H^0\), which should be plausibly positive for a hole-doped insulator although this is not trivial to show analytically \[\mathbf{q}\]. For a single carrier we also get for \(q \to 0\) \((\rho^q)_{\ell\ell'} = 1\) which is an alternative requirement for a well defined quasiparticle. We note also that the second term in Eq.\((26)\) does not contribute since \((\rho^q)_{00} = 0\) if \(x\) and \(y\) are symmetry directions of the \(D\) tensor.

B. 1D systems

Naturally one cannot discuss Hall effect and \(R_H^0\) in a strictly 1D system but it is instructive to consider relations which follow from our analysis for \(D^0\) and \(\kappa^0\). We assume here that the correlated electron system behaves as a Luttinger liquid with gapless charge excitations characterized by a linear dispersion for \(q \to 0\),

\[
\epsilon_{\ell\ell'} = E_{\ell\ell'}(q) - E_0 \sim v_c q. \tag{44}
\]

The counting of states \(|\ell\rangle\) is then as for electron-hole excitations in the normal Fermi liquid.

Assuming that Eqs.\((31),(33)\) behave regularly as \(q \to 0\), we can replace \((j_y^q)_{0\ell\ell'} \to j_e\) and \((\rho^q)_{0\ell\ell'} \to r_c\). From Eq.\((32)\) it follows also that \(j_e = v_c r_c\) and we get (taking into account also the spin degeneracy),

\[
D^0 = \frac{j_y^2}{\pi v_c} = \frac{r_c^2 v_c^2}{\pi}, \quad \kappa^0 = \frac{2r_c^2}{\pi v_c}. \tag{45}
\]

These expressions are in agreement with the phenomenology of the Luttinger liquids \[\mathbf{q}\] where we can identify the renormalization factor \(r_c\) with the density exponent \(K_p = r_c^2\). Although there is another gapless branch of spin excitations, we note that this does not enter the quantities as the charge stiffness \(D^0\) and the charge compressibility \(\kappa^0\). Our analysis is at \(T = 0\), it is easy to argue that for low \(T\) specific-heat coefficient we get \(C_V \propto 1/v_c\).
V. FERMII LIQUID

Let us now consider as an illustration of the above formalism a Fermi system characterized by gapless charge excitations with a linear dispersion (for \( q \to 0 \)),

\[
\epsilon_{\tilde{m}} = E_{\tilde{m}}(q) - E_0 = v(k) \cdot q ,
\]

corresponding to electron-hole excitations and a Fermi surface \( k_F \). The states \( |\tilde{m}\rangle \) are then determined as electron-hole excitations in the normal Fermi liquid so at given \( q \) they are characterized by \( k \in \mathbf{F}_\mathbf{S}_q \). For the general direction \( \mathbf{e}_\beta = q/q \) the states are given by \( k = k_F + k e_\beta \) and \(-q < \tilde{k} < 0\), where the latter condition is satisfied only along half of the Fermi surface.

Assuming that the fermionic character of such excitations (with spin), we can write the sums over excited states explicitly for the thermodynamic limit taking into account spin degeneracy and \( q \to 0 \),

\[
\frac{1}{N} \sum_{\tilde{m}} = \frac{1}{N} \sum_{k \in \mathbf{F}_\mathbf{S}_q} \frac{2q}{(2\pi)^2} \oint_{k_\beta < 0} \frac{dk_F}{v(k)} \epsilon_{\mathbf{e}_\beta}(k) ,
\]

again restricting our analysis to 2D systems.

Here we note that in general the operators \( j^\alpha_\beta, \tau^\alpha_{\alpha\beta}, \rho^\alpha \) (at \( B = 0 \)) can be represented as

\[
\begin{align*}
    j^\alpha_\beta &= \sum_{k,s} v^{\alpha}_k c_{k+q/2,s} c_{k-q/2,s} , \\
    \tau^\alpha_{\alpha\beta} &= \sum_{k,s} v^{\alpha\beta}_k c_{k+q/2,s} c_{k-q/2,s} , \\
    \rho^\alpha &= \sum_{k,s} v^\alpha_k c_{k+q/2,s} c_{k-q/2,s} ,
\end{align*}
\]

where \( v_k = \partial k_\beta / \partial k \) and \( \tau_\beta = \partial^2 k_\beta / \partial k \partial k \).

In the following we can consider as a test noninteracting electrons with dispersion \( \epsilon_k \), where the relevant excited states are

\[
|\tilde{m}\rangle = c_{k-q/2,s} c_{k+q/2,s}|0\rangle .
\]

Let us first treat \( D^\alpha_{\alpha\alpha} \), Eq.(50),

\[
D^\alpha_{\alpha\alpha} = \frac{2q}{(2\pi)^2} \oint_{k_\beta < 0} \frac{dk_F}{v(k)} |j^\alpha_\beta|_{0\tilde{m}}^2 \epsilon_{\tilde{m}} = \frac{1}{(2\pi)^2} \oint \frac{dk_F}{v(k)} |j^\alpha_\beta|_{0\tilde{m}}^2 .
\]

For \( q \to 0 \) the result must be independent of \( q \) so it is plausible that

\[
(j^\alpha_\beta)_{0\tilde{m}} \to j_\alpha(k)
\]

depends only on \( k \in k_F \), and

\[
D^\alpha_{\alpha\alpha} = \frac{1}{(2\pi)^2} \oint \frac{dk_F}{v(k)} |j_\alpha(k)|^2 .
\]

For noninteracting fermions the expression \( (j^\alpha_\beta)_{0\tilde{m}} \) is straightforward since we know from Eqs.(48)-(49) that \( j_\alpha(k) = v_\alpha(k) = v_\alpha^0 \).

In the same way we can also argue that \( (\rho^\alpha)_{0\tilde{m}} \to r(k) \), which can be concluded from Eq.(50),

\[
\kappa^\alpha = \frac{q}{\pi^2} \oint_{k_\beta < 0} \frac{dk_F}{v(k)} \epsilon_{\mathbf{e}_\beta}(k) \frac{|(\rho^\alpha)_{0\tilde{m}}|^2}{\epsilon_{\tilde{m}}} = \frac{1}{2\pi^2} \oint \frac{dk_F}{v(k)} |(\rho^\alpha)_{0\tilde{m}}|^2 = \frac{1}{2\pi^2} \oint \frac{dk_F}{v(k)} (\rho^\alpha)^2 (k) .
\]

Furthermore for noninteracting fermions we get \( (\rho^\alpha)_{0\tilde{m}} = r(k) \).

Let us turn to the discussion of \( \Lambda_{yx} \). Matrix elements \( (d^x_y)_{\tilde{n}\tilde{m}} \) within a Fermi liquid are (for chosen \( q \) direction) expected to depend only on \( k \) along the Fermi surface, so we can replace \( (d^x_y)_{\tilde{n}\tilde{m}} \to d_{xy}(k) \) and

\[
\Lambda_{yx} = \frac{1}{8\pi^2} \oint \frac{dk_F}{v(k)} j_y(k) v_y(k) d_{xy}(k) .
\]

Taking into account Eq.(50) and that the role of \( \tilde{\theta} \) is to shift \( k \) we can also relate,

\[
\frac{\partial}{\partial x} (j^x_y)_{0\tilde{m}} \to \frac{\partial}{\partial k} j_x(k) .
\]

Eq.(50) can therefore be written as

\[
\Lambda_{yx} = \frac{1}{8\pi^2} \oint \frac{dk_F}{v(k)} j_y(k) \left[ v_y(k) \frac{\partial}{\partial k} j_x(k) - v_x(k) \frac{\partial}{\partial k} j_y(k) \right]
\]

At this stage we are unable to put also the second term in analogous form as the first one. Still the expression is very similar to the symmetric one,

\[
\tilde{\Lambda}_{yx} = \frac{1}{8\pi^2} \oint \frac{dk_F}{v(k)} j_y(k) v_y(k) \times \mathbf{e}_B \cdot \nabla j_x(k) ,
\]

which is formally equivalent to the Boltzmann expression within the relaxation-time approximation \([15, 16]\). A clear advantage of the symmetric expression is that the required \( xy \) symmetry \( \Lambda_{yx} = -\Lambda_{xy} \) is evident, since Eq.(50) can be represented as

\[
\tilde{\Lambda}_{yx} = \frac{1}{16\pi^2} \oint [dj(k) \times j(k)] \cdot \mathbf{e} = \pm \frac{S_j}{8\pi^2} ,
\]

where \( S_j \) is the area spanned by the vector \( j(k_F) \).

Again testing with the case of noninteracting fermions we note that in Eq.(50) the second term is

\[
\frac{1}{q} (j^x_y)_{\tilde{n}\tilde{m}} \to v_x(k) \frac{\partial}{\partial k} v_x(k) .
\]
therefore we reproduce the usual semiclassical expression \[16\] for \( \Lambda_{yx} \), Eqs. (53),(58), up to a constant (relaxation time) which anyhow cancels out in \( R_H^0 \), Eq. (12). It should be also reminded that for noninteracting fermions on a bipartite lattices with nearest neighbor hopping the term (59) vanishes since we have \( v_\alpha (k_\alpha) \).

A. Quasi-1D systems

Let us assume a very anisotropic Fermi liquid with a dispersion large only in the \( z \) direction and consequently also a nearly flat Fermi surface with \( |k_F| \sim k_0 \). It is plausible that for large anisotropy Eq. (54) can be decoupled as

\[
\Lambda_{yx} \sim d_{xx}(k_F) \frac{1}{(2\pi)^2} \int \frac{dk_F}{v(k)} j_y(k) j_y(k) .
\]

(60)

It follows also that

\[
D_{y\beta}^0 = \frac{1}{(2\pi)^2} \int \frac{dk_F}{v(k)} j_y^2(k) , \quad D_{xx}^0 \sim D .
\]

(61)

Now we can use relations (56),(57) for a Fermi liquid in the limit \( q \to 0 \),

\[
\frac{\partial D_{xq}^q}{\partial \mu} = \frac{1}{2\pi^2} \int \frac{dk_F}{v(k)} r(k)d_{xx}(k) .
\]

(62)

For a nearly flat Fermi surface we can replace \( d_{xx}(k_F) \sim d_{xx}(k_F) \) and we get

\[
\frac{\partial D_{xq}^q}{\partial \mu} \to \frac{\partial D}{\partial \mu} = d_{xx}(k_F) \frac{1}{2\pi^2} \int \frac{dk_F}{v(k)} r(k) ,
\]

(63)

where we have also assumed that taking the derivative \( \partial D/\partial \mu \) is regular for \( q \to 0 \). So finally we can express \( R_H^0 \) as \( (e = -e_0) \),

\[
R_H^0 = -\frac{A}{e_0 D} \frac{\partial D}{\partial \mu} ,
\]

\[
A = \int \frac{dk_F}{v(k)} v^2(k) \int \frac{dk_F}{v(k)} v_y(k) j_y(k) / \int \frac{dk_F}{v(k)} r(k) \int \frac{dk_F}{v(k)} j_y^2(k) .
\]

(64)

For a quasi-1D system we expect that \( r(k_F) \sim r_F \), \( v(k_F) \sim v_F \) and therefore \( j(k_F) = r_F v(k_F) \) and consequently \( A \sim 1 \). Hence we have reproduced in this case the desired expression (1).

B. Isotropic Fermi liquid

Although the tight binding model, as introduced initially in Eq. (3), does not lead to an isotropic Fermi surface, an isotropic Fermi liquid can still be of interest for illustration and can also emerge in specific cases. We assume here that \( j(k) = j(k) e_k \) and \( v(k) = v(k) e_k \), so that Eqs. (32),(36) lead to

\[
D_{\alpha\alpha}^0 = \frac{k_F^2 j^2}{4\pi v_F} , \quad \Lambda_{yx} = \frac{j^2}{4\pi} .
\]

(65)

and

\[
R_H^0 = -\frac{4\pi v^2}{e_0 k_F^2 j^2} = -\frac{1}{e_0 n_F r_F^2} ,
\]

(66)

where \( n_F = k_F^2/2\pi \) is the effective density of electrons as determined by the volume of the Fermi surface.

VI. DISCUSSION

The theory of the Hall constant in systems with strongly correlated electrons is evidently a difficult subject. In spite of its relevance for the intensively investigated anomalous properties of cuprates, there has been so far no consensus on the behavior and even less in the appropriate formalism for an analytical evaluation of the \( R_H(\omega) \).

It is clearly an advantage to deal with the system at \( T = 0 \) since here the transport (reactive) Hall constant \( R_H^0 \) is well defined but does not involve any scattering or dissipation. One could hope that such \( R_H^0 \) remains a reasonable approximation for \( R_H(T) \) at finite but small \( T > 0 \). This is for example the case for normal metals and semiconductors where within the approximation of uniform (in \( k \)) but \( T \) dependent relaxation rate \( \tau(T) \) the latter cancels out and finally \( R_H(T) \sim R_H^0 \).

The central quantity in our approach for \( R_H(\omega) \) is the off-diagonal stiffness \( \Lambda_{yx} \) which plays analogous role as the charge stiffness \( D_{\alpha\alpha} \) in the diagonal optical conductivity \( \sigma_{\alpha\alpha}(\omega) \). We show in Sec. II that \( \Lambda_{yx} \) can be expressed in terms of matrix elements involving solely lowest excited state (at \( B = 0 \)) which is a conceptual and technical simplification, which is also well adapted for application to a broader class of Fermi liquid systems. For a Fermi system with well defined Fermi surface and gapless electron-hole excitations we also find a formal correspondence (apart from some ambiguities with the second term in Eq. (50)) of the expression for \( \Lambda_{yx} \) with the one in the relaxation-time approximation. The main difference in correlated system is that effective quantities \( v(k) \) and \( j(k) \) are not directly related.

From the general formalism in Sec. II it is clear that there is intimate relation between \( \Lambda_{yx} \) and the matrix elements of the stiffness operator, Eqs. (22),(23). More directly we can express \( R_H^0 \) with the \( D(n) \) itself in the case of quasi-1D correlated system, where we recover (under certain restrictions) the expression (1), derived quite generally in the slow limit (first \( \omega = 0 \), then \( q \to 0 \)). The Hall response of such quasi-1D systems is of direct experimental interest, in particular recently in connection with the apparent controversies in 1D conductors [13] as
well as with the striking vanishing of the Hall constant in the stripe phase of cuprates \cite{19, 20}. Since strongly correlated quasi-1D systems are not expected to be singular one can expect that the relation \( (1) \) remains qualitatively valid even for a broader class of strongly correlated electrons.

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