Hall constant of strongly correlated electrons on a ladder

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The Hall constant \( R_H\) in a tight-binding model of correlated electrons on a ladder at \( T = 0\) is expressed in terms of derivatives of the ground state energy with respect to external magnetic and electric fields. This novel method is used for the analysis of the \( t\)-\( J\) model on finite size ladders. It is found that for a single hole \( R_H\) is hole-like and close to the semiclassical value, while for two holes it can vary with ladder geometry. In odd-leg ladders, \( R_H\) behaves quite regularly changing sign as a function of doping, the variation being quantitatively close to experimental results in cuprates.

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The Hall response in materials with strongly correlated electrons remains one of the properties least understood theoretically. The subject has been stimulated by experiments in superconducting cuprates, revealing anomalous doping and temperature dependence of the Hall constant \( R_H(T)\) in the normal metallic state. For instance, it is well established that the Hall effect is hole-like, \( R_H > 0\), in materials with a low density of holes \( n_h\), introduced by doping the reference antiferromagnetic (AFM) insulator. The clearest realization is \( La_{2−x}Sr_xCuO_4\) (LSCO), where the doping \( x\) can be directly related to the concentration of mobile holes per unit cell \( n_h = x\) and the semiclassical result \( R_H = 1/n_h e_0\) seems to be obeyed at lowest \( T > T_c\) and at low doping \( T \ll T_c\).

Theoretical attempts to calculate the Hall effect in models of strongly correlated electrons resulted in quite controversial conclusions. Even for weak correlations \( J \ll \epsilon_0\) or for the problem of a single carrier in a Mott-Hubbard insulator \( J > \epsilon_0\), the analysis of the Hall response is fairly involved. In more recent investigations relevant to cuprates, the dynamical Hall constant \( R_H(\omega)\) has been studied within linear response theory for the \( t\)-\( J\) and Hubbard model, analytically by high-\( \omega\), \( T\) expansion \( J > \epsilon_0\) and numerically via exact-diagonalization studies of small systems \( J > \epsilon_0\). The obtained results are quite consistent for the high-frequency quantity \( R_H^* = R_H(\omega \to \infty)\), showing at high \( T\) a transition from a hole-like, \( R_H^* > 0\), to an electron-like, \( R_H^* < 0\), at a finite crossover \( n_h^* \sim 1/3\).

For the most interesting d.c. limit \( R_H = R_H(\omega = 0)\) the majority of results obtained for 2D systems at low doping and \( T \to 0\) indicate \( R_H < 0\), instead of the expected hole-like behavior \( R_H > 0\). On the other hand, one of the present authors \( J > \epsilon_0\) recently showed that for a single hole doped into a 2D AFM at \( T = 0\) the result should be the semiclassical one with \( R_H > 0\).

From another perspective and stimulated by synthesis and experiments on novel cuprates, models of interacting electrons on ladder systems have also been extensively studied in recent years \( J > \epsilon_0\). The idea is that ladders with a variable number of legs can offer a broader insight into the behavior of correlated electrons and thus can lead to an understanding of the more challenging 2D systems. Again, results for the Hall response \( R_H(\omega)\) at low doping obtained through linear response theory reveal a quite puzzling, electron-like, \( R_H < 0\) behavior.

Our aim in this work is to formulate and calculate the Hall constant as a ground state \( (T = 0)\) property for a tight-binding model with a ladder geometry. This is possible due to the finite transverse width of the system that, in contrast to an infinite 2D (or higher D) system, does not require a relaxation mechanism to describe a proper transport regime. Such a formulation allows for a more transparent calculation of \( R_H\) and in particular the determination of its sign \( J > \epsilon_0\). In the following, we apply this method to the \( t\)-\( J\) model on a ladder. Via a numerical analysis of small systems, we investigate \( R_H\) for few holes \( N_h = 1, 2\) and a finite concentration of holes \( n_h > 0\) introduced into an AFM correlated spin background.

Let us consider the simplest single-band tight-binding model of interacting fermions on a ladder geometry with \( M\) legs in the \( y\) direction, \( L\) rungs in the \( x\) direction. Periodic boundary conditions \( (p.b.c.)\) are assumed in the \( x\) direction and unit-cell length \( a_0 = 1\). To analyze the Hall response, the following additional ingredients need to be incorporated into the model:

a) a finite transverse electric field \( E_y = E \neq 0\) has to be taken into account,
b) a homogeneous magnetic field \( B\) perpendicular to the ladder, introduced via the Peierls substitution. In the Landau gauge \( A = B(−y,0)\), only the phases of hopping integrals in the \( x\) direction, \( H_x\), are modified by a phase \( \varphi = e_0B \ (h = 1)\). We also assume that the interaction term \( H_{int}\) is not influenced neither by \( A\) nor by \( E\).

c) a steady electric current density \( j = j_x\) is induced in the ground state by piercing a closed ladder in the \( y\) direction with a flux \( \Phi\), modifying the hopping term by a phase \( \theta = e_0\Phi/L\).
The tight-binding model can be thus written as,

\[
H = H_x + H_y + H_\Delta + H_{int}
\]

\[
H_x = -t \sum_{m=1}^{M} \sum_{is} e^{i(m-\hat{m})\varphi - \theta}(c_{m,i+1,s}^{\dagger} c_{m,i,s} + H.c.),
\]

\[
H_y = -t' \sum_{m=1}^{M-1} \sum_{is} (c_{m+1,i,s}^{\dagger} c_{m,i,s} + H.c.),
\]

\[
H_\Delta = \Delta \sum_{im}(m - \hat{m})n_{mi},
\]

where \( \Delta = e_0 \mathcal{E}, \hat{m} = (M+1)/2 \) and \( H_{int} \) will be chosen later on.

The idea is to study the ground state energy \( E(\theta, \Delta, \varphi) \) of the system as a function of \( \Delta, \theta, \varphi \) in order to evaluate the Hall constant \( R_H \),

\[
R_H = \frac{e_0}{jB} \frac{\Delta}{\Delta \varphi}.
\]

We use the fact that the electric current density \( j \) and polarization density \( P = P_\theta \) in the ground state \( |0\rangle \) can be evaluated via derivatives of the energy \( E(\theta, \Delta, \varphi) \) using the Feynman-Hellmann relations,

\[
j = \frac{e_0}{N} \frac{\partial E}{\partial \theta}, \quad P = \frac{e_0}{N} \frac{\partial E}{\partial \Delta},
\]

where \( N = LM \) denotes the number of lattice points.

In the absence of the magnetic field, \( \varphi = 0 \), we use as starting point an equilibrium and nonpolar ground state with \( j = 0 \) and \( P = 0 \). Such a ground state might correspond to finite values \( \theta_0 \) and \( \Delta_0 \). In ladders one expects (for a nondegenerate ground state) \( \Delta_0 = 0 \) by symmetry. On the other hand, in finite systems, in general we find \( \theta_0 \neq 0 \). This can be considered as a finite size effect, since in the thermodynamic limit \( L \to \infty \) no macroscopic current is expected in the ground state and so \( \theta_0 \to 0 \) (for a particular study of finite-size scaling of \( \theta_0 \) see e.g. Ref. [12]). Taking a proper starting \( \theta_0 \) in the following calculations is however crucial for obtaining a sensible result.

Next, to simulate the Hall effect we analyze systems with small but finite current \( j \neq 0 \) imposed by a finite \( \tilde{\theta} \), magnetic field imposed by a \( \varphi \neq 0 \) and choosing a \( \Delta \neq 0 \) so that the system remains nonpolar, \( P = 0 \). Hence we have to study the variation of \( E(\theta_0 + \tilde{\theta}, \Delta, \varphi) \) for small \( \tilde{\theta}, \Delta, \varphi \). It is enough to consider a Taylor expansion up to \( 3^{rd} \) order, simplified by invoking: (i) the symmetry of the current operator \( j_0 = \frac{e_0}{N} \frac{\partial H}{\partial \theta}(\theta \neq 0, \varphi = 0) \) under reflection \( (\Delta \to -\Delta) \) and, (ii) the reflection antisymmetry of the diamagnetic current \( j_0^\ast = \frac{e_0}{N} \frac{\partial \Delta}{\partial \varphi}(\theta \neq 0, \varphi = 0) \) and the polarization operator \( \tilde{P} = -\frac{e_0}{N} \frac{\partial H}{\partial \Delta}(\theta = 0, \varphi = 0) \).

This leads to:

\[
E = E^0 + \frac{1}{2} E^0 \tilde{\theta} \Delta + \frac{e_0}{N} \frac{\partial E^0}{\partial \Delta} \Delta^2 + E^0 \tilde{\varphi} \varphi + \frac{1}{2} E^0 \tilde{\varphi} \varphi \Delta + \frac{1}{2} E^0 \Delta \hat{\varphi} \Delta^2 + \frac{1}{2} \frac{e_0}{N} \frac{\partial E^0}{\partial \varphi} \tilde{\varphi}^3 + \cdots.
\]

The superscript zero indicates derivatives at equilibrium (at \( \varphi = 0 \)). From Eqs. (3,4) and to leading order, \( j \) is given by

\[
j = \frac{e_0}{N} E^0_\theta \tilde{\theta},
\]

while the Hall field \( \Delta \) is set by the condition that \( P = 0 \) even in the presence of finite \( \tilde{\theta}, \tilde{\varphi} \),

\[
E^0_\Delta \Delta + E^0_\Delta \varphi + E^0_\varphi \varphi + E^0_\varphi \tilde{\theta} \Delta = 0.
\]

Retaining terms linear in \( \varphi \) and \( \tilde{\theta} \) we can express \( \Delta \) as

\[
\Delta = \Delta_\varphi + \Delta_j = \frac{E^0_\Delta}{E^0_\varphi} \varphi - \frac{\tilde{E}^0_\Delta}{E^0_\varphi} \tilde{\theta} \Delta
\]

\[
\tilde{E}^0_\Delta \Delta = \frac{E^0_\Delta}{E^0_\varphi} \frac{E^0_\Delta}{E^0_\varphi} \tilde{\theta} \Delta.
\]

We are interested in the second term, i.e. in \( \Delta_j \) induced by finite \( \tilde{\theta} \) and related \( j \). We note also that \( \tilde{E}^0_\Delta \Delta \) can be expressed simply as the derivative taken at the origin \( \Delta_0 = 0 \) shifted to \( \Delta \). Inserting \( \Delta_j \) from Eq.(7) and \( j \) from Eq.(8) into Eq.(8), we obtain the expression

\[
R_H = \frac{N \tilde{E}^0_\Delta \Delta}{e_0 E^0_\varphi E^0_\varphi}.
\]

This is a central result in this work. The main advantages of the new approach are: (i) Eq.(8) requires the knowledge of only the ground state energy, (ii) the condition for \( j = 0 \), \( P = 0 \) in the reference ground state of finite size systems is much more transparent.

Now we will show how this formulation is related to the linear response theory for the particular case of ladders at \( T = 0 \), where \( R_H \) is evaluated via the dynamic (in general complex) \( \tilde{R}_H(\omega) \),

\[
\tilde{R}_H(\omega) = -\frac{1}{B} \frac{\sigma_{yz}(\omega)}{\sigma_{xz}(\omega)} \frac{e_0}{N} \frac{\partial H(\omega)}{\partial \varphi}.
\]

\[
\sigma_{\alpha\beta}(\omega) = \frac{i e_0^2 \omega}{N} \int_0^\infty dt d\omega [(\tilde{\gamma}_\alpha(t), \tilde{\gamma}_\beta)],
\]

\[
\tilde{\gamma}_{\alpha}(\omega) = \frac{i e_0^2}{\omega N} \int_0^\infty dt d\omega \frac{e_0}{N} \frac{\partial H(\omega)}{\partial \alpha} (\tilde{\gamma}_\alpha(t), \tilde{\gamma}_\beta).
\]

\[
\sigma_{xx}(\omega \to 0) = \frac{2i e_0^2}{\omega} D_{xx} \equiv \frac{i e_0^2}{\omega} E_{\theta \theta}.
\]

where \( D_{xx} \) denotes the charge stiffness [13,4]. On the other hand, in the \( y \) direction the polarizability \( \chi_{yy}(\omega \to 0) \) is finite due to open boundaries. Using the relation \( \tilde{\gamma}_\beta = d\tilde{\theta}/dt \), we get from Eq.(9)
The off-diagonal \( \sigma_{yx} (\omega = 0) \) can be written as

\[
\sigma_{yx}(\omega = 0) = -iN \int_0^\infty dt \langle [\hat{P}(t), \hat{j}] \rangle = 2N \sum_m \frac{\langle 0| [\hat{\rho}m|0] \rangle}{E_0 - E_m} = -e_0 \frac{\partial \langle 0|\hat{j}|0 \rangle}{\partial \Delta} = -\frac{e_0^2 E_{\theta\Delta}}{N},
\]

(12)

where the ground state \( |0 \rangle \), excited states \( |m \rangle \) as well as \( E_{\theta\Delta} \) refer to \( \varphi \neq 0 \) but \( \Delta = 0 \). Taking into account that \( E_{\theta\Delta} \propto \varphi \) and inserting relations (10-12) into Eq.(9) we recover the expression (8), provided that \( E_{\theta\Delta}^0 = 0 \). The equivalence for the case \( E_{\Delta\varphi}^0 \neq 0 \) can also be obtained if one calculates the linear response \( \sigma_{yx} \) in Eq.(12) not at \( \Delta = 0 \), but rather at the proper \( \Delta = \Delta_\varphi \).

\( \varphi \)From linear response theory we observe that the existence of the simple expression Eq.(8) is subject to the presence of the restricted geometry which implies a finite \( \sigma_{yx}(\omega = 0) \) as well as a finite \( \sigma_{xx}(\omega)\sigma_{yy}(\omega) \) for \( \omega \to 0 \). Both quantities would diverge for \( T = 0 \) at the 2D limit \( (M \to \infty) \), although \( R_H(\omega \to 0) \) is expected to remain well defined and bounded (3).

Let us first test the method for noninteracting electrons on a two-leg \((M = 2)\) ladder. It is here easy to find the single-electron eigenenergies \( \epsilon_{\pm}(k, \theta, \Delta, \varphi) \), referring to the upper and lower band. At \( T = 0 \), states in both bands are occupied for \( \epsilon_{\pm} < \epsilon_F \), and the result follows from Eq.(8),

\[
R_H = \frac{\tau^+ - \tau^-}{e_0(\tau^- + \tau^+)(n_e^- - n_e^+)},
\]

(13)

where \( n_e^\pm \) are electron densities in both bands and \( \tau^\pm = 4t \sum_{|k| < k_F} \cos k \). Note that Eq. (13) reduces to plausible expressions: a) the semiclassical result \( R_H = -1/n_e e_0 \) for an empty upper band, \( n_e^+ = 0 \), and b) \( R_H = 1/n_e e_0 \) for a filled lower band \( n_e^- = 1 \), where \( n_e = 1 - n_e^+ = 2 - n_e^- \) is the density of holes in the upper band.

Now, we illustrate the method and expected as well as anomalous features of the Hall response in correlated systems on a study of the isotropic t-J model \((t' = t)\). The interaction term in Hamiltonian (1) describes AFM exchange interaction between fermionic spins on neighboring sites \( j = (m, i) \),

\[
H_{int} = J \sum_{\langle ij \rangle} \hat{S}_j \cdot \hat{S}_{j'},
\]

(14)

and fermionic operators in the kinetic energy term are replaced by projected ones, forbidding a double occupancy of sites. Note that the projection does not influence the general formalism, Eqs(8-11).

To obtain \( E(\theta, \Delta, \varphi) \) and consequently \( R_H \) in finite size ladders we employ the Lanczos diagonalization technique. For a particular system with given \( M, L \) and fixed number of holes \( N_h \) we first find the energy minimum at the equilibrium \( \theta_0 \) and then calculate numerically at this point derivatives \( E_{\Delta\varphi}^0, E_{\theta\theta}^0, E_{\theta\Delta\varphi}^0, E_{\theta\Delta\varphi}^0 \). Then \( R_H \) is evaluated using relations (3).

In Fig. 1a,b we show results for the dimensionless \( r_H = e_0 R_H/N \) in the case of a single hole \( N_h = 1 \) on \( M = 2 \) and \( M = 3, 4 \) ladders, respectively, of varying length and as a function of \( J/t \). Note that the semiclassical result in this case would be \( r_H = 1 \). We should note that in general we find here \( \theta_0 \neq 0, \pi \). Moreover the influence of \( \Delta \varphi \neq 0 \) is essential since \( E_{\Delta\varphi}^0 \) differs from \( E_{\theta\Delta\varphi}^0 \) significantly. E.g., for \( M = 2 \), in the most relevant regime \( J < t \) both quantities can even be of a different sign. We notice that results for different \( L \)'s are quite consistent. \( J = 0 \) is a special case with a ferromagnetically polarized ground state, \( S^{tot} = (N - 1)/2 \) and hence \( r_H = 1 \). Also, as Fig. 1 shows, for \( J > 0 \) \( R_H \) is hole-like with \( r_H \geq 1 \). This means that the behavior is very close to the semiclassical one (3), but the deviation from the latter is finite (although smaller for larger \( M \)) and seems to persist also for \( L \to \infty \).

![FIG. 1. Dimensionless Hall constant \( r_H = e_0 R_H/N \) vs. \( J/t \) for a single hole on ladders of different lengths \( L \) with: a) two legs and, b) three and four legs.](image-url)

Results for two holes are presented in Fig. 2. At very low doping, \( n_h \ll 1 \), one might expect that in the thermodynamic limit holes behave as independent particles so that \( r_H \sim 1/N_h \). This is definitely not the case for \( M = 2 \), where in the majority of the parameter regime we even find \( r_H < 0 \), consistent with Ref. [1]. It seems that this phenomenon is related to the existence of a spin gap in \( M = 2 \) ladders and quite pronounced binding of holes into pairs (10). Results appear more regular for \( M > 2 \). Conclusions quite consistent with the semiclassical \( r_H \sim 1/2 \) are obtained for the \( M = 3 \) and \( M = 4 \) ladders. It is well known that odd-leg ladders do not
show a spin gap [10], so this can serve as an explanation for the essential difference between the $M = 3$ and $M = 2$ case. For $M = 4$, a small spin gap is expected in undoped ladder [10], however its effect on $r_H$ is not visible, at least not for reachable $L$.

In systems with more holes, $N_h > 2$, and available $N \leq 20$ we are dealing already with a substantial doping $n_h$. In Fig. 3 we show results for the doping dependence $R_H(n_h)$. We concentrate on a more regular three-leg ladder, where even-odd effects in $N_h$ are not pronounced. Shown are data for two systems, $5 \times 3$ and $6 \times 3$. Results for both systems are in general quite consistent, with deviations appearing only in the regime $n_h \sim 0.2$ where in particular the value for $N_h = 4$ on a $6 \times 3$ system appears to be irregular, probably a finite-size effect related e.g. to a close-shell configuration.

The interpretation of Fig. 3 is straightforward in two regimes. For a nearly empty band $n_h \lesssim 1$, $n_e = 1 - n_h \gtrsim 0$ we recover the semiclassical result, $e_0 R_H = -1/n_e$. Analogous, but only approximate, is the hole-like behavior for low doping $n_h \ll 1$ where $e_0 R_H \sim 1/n_h$. The behavior is very asymmetric between the hole and the electron side. The change from a hole-like $R_H > 0$ to an electron-like $R_H < 0$ appears (with the largest scattering of results in this regime) at $n_h^* \sim 0.27$. Our value for the crossover $n_h^*$ is close to the crossover in $R_H = 1/4n_h - 1/(1 - n_h) + 3/4$ (in 2D and $T \to \infty$) at $n_h^* \sim 1/3$. [3] In spite of similar values for $n_h^*$ and a quantitative agreement for $n_h > 0.3$, $R_H$ (also plotted in Fig. 3) deviates at low doping values by factor of 4 from the semiclassical result.

Although we are dealing with a ladder system, we expect that results for odd-leg ladders would be very analogous to 2D systems. It is therefore not surprising that our results for $R_H(n_h)$ are both qualitatively as well quantitatively close to experimental ones for LSCO (doping range $0 < x < 0.35$), where values shown in Fig. 3 are taken at $T = 100 \, K$ [2]. We note that experimentally the crossover appears at $x \sim 0.3$ and at low doping, data are consistent with the semiclassical $R_H \sim 1/n_h e_0$.

In conclusion, we have introduced a novel method which allows the evaluation of the d.c. Hall constant at $T = 0$ in correlated systems with a ladder geometry solely from the ground state energy. Since the behavior of ladder systems is in many respects analogous to 2D systems the method can be used to approach the anomalous and theoretically controversial $R_H$ in cuprates. Our numerical results emerging from odd-leg ladders are indeed surprisingly close to experiments in LSCO.

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