Memory-function approach to the Hall constant in strongly correlated electron systems

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The anomalous properties of the Hall constant in the normal state of high-T_c superconductors are investigated within the single-band Hubbard model. We argue that the Mori theory is the appropriate formalism to address the Hall constant, since it aims directly at resistivities rather than conductivities. More specifically, the frequency-dependent Hall constant decomposes into its infinite frequency limit and a memory-function contribution. The latter naturally introduces a second time scale that is identified with the spinon relaxation time of Anderson within the t-J model. This provides us with a phenomenological understanding of the interplay between the frequency and temperature dependence of the Hall constant for frequencies below the Mott-Hubbard gap. As a first step, both terms of R_H are calculated perturbatively in U and on an infinite dimensional lattice, where U is the correlation strength. If we allow U to be of the order of twice the bare bandwidth, the memory-function contribution causes the Hall constant to change sign as a function of doping and to decrease as a function of temperature. In the strong correlation regime, $U \gg t$ (t is the hopping amplitude), the memory function is calculated via its moments and shown to project out the high-energy scale U. This causes the Hall constant to decrease by a factor $(1+\delta)/2$ (δ indicates doping), when the frequency is lowered from infinity to values within the Mott-Hubbard gap. Finally, it is outlined how the Hall constant may be calculated in the low-frequency regime. [S0163-1829(97)03706-5]

I. INTRODUCTION

Since the discovery of high-T_c superconductors ten years ago, the anomalous properties of their normal state have been the subject of intensive theoretical work. It is widely believed that a model of strongly correlated electrons already captures the basic ingredients of the relevant physics. In these models, the correlations are represented by a strong local interaction U. However, a coherent description of *all* anomalous properties on the basis of such a model is still lacking. The main problem is that exact calculations are generally feasible only in a small parameter regime and that most approximation schemes fail in capturing *all* aspects which are supposed to be important.

The Hall constant is especially hard to describe. One reason for this is that the Hall conductivity contains a three-point correlation function after it has been expanded to first order in the magnetic field. Then, the calculation of vertex corrections is a tough problem which, to our knowledge, has been attempted only in the case of a Fermi liquid and to leading order in the quasiparticle damping.[1] Moreover, since the frequency-dependent Hall constant is given as a quotient of conductivities, the limit $\omega \to 0$ may be precarious due to resonances like the Drude peak. A more technical peculiarity of the Hall effect is due to the fact that the magnetic field is introduced via a vector potential which, formally, breaks the symmetry with respect to lattice translations. But even in the simplest case of a Bloch-Boltzmann description, the temperature dependence of the Hall constant may be difficult to reproduce, because the relaxation time cancels once it is assumed to be independent of momentum.

The measurements of the Hall constant in high-T_c materials[2] reveal two major anomalous dependences: on temperature and on doping. Both cannot be understood within conventional band theory. For noninteracting tight-binding electrons on a two-dimensional square lattice, the Hall constant changes sign at half filling as the Fermi surface changes its shape from electronlike to holelike. In contrast, the Hubbard model in the large-U limit exhibits an additional sign change below half filling which is purely due to correlations.[3,4] In addition, in the limit $\delta \to 0$, i.e., near half filling, the Hall constant diverges according to a $1/\delta$ law.[3,4] These properties are supposed to account for the doping dependence observed in, e.g., $La_{2-x}Sr_xCuO_4$.[5,6] As for the anomalous temperature dependence of the Hall constant, the most striking features are: firstly, a strong decrease which is, in some cases, as fast as $1/T$;[2] secondly, the lack of saturation above a fraction of the Debye temperature, typically $\sim 0.2-0.4T_D$,[7,8] in contrast to what is expected in a Fermi-liquid description with weak electron-phonon coupling;[9] and thirdly, a quadratic dependence of the inverse Hall angle on temperature for not too large doping levels.[8,10,11] In a Fermi liquid, the temperature dependence arises from an anisotropic relaxation time.[7,9] If we assume scattering off phonons to be the main inelastic process, a temperature dependence is conceivable only below a certain temperature scale: Then, a sufficiently anisotropic Fermi surface causes the scattering to be confined to those regions of the Fermi surface, where small momentum transfers are possible. For high enough temperatures, this kinematic restriction is lifted and the scattering becomes isotropic, thus leading to a cancellation of the relaxation time. The crossover temperature is given by $\sim 0.2-0.4T_D$. The universally observed decrease of the Hall constant as a function of temperature in almost all high-T_c compounds up to temperatures clearly beyond this temperature scale must therefore be due to electronic correlations as well.

In the following, we investigate the Hall effect on the basis of the simplest model of strongly correlated electrons, namely the single-band Hubbard model on a hypercubic lat-

tice in d dimensions with nearest-neighbor hopping. This model, along with Mori's formalism used to represent the Hall constant, is introduced in Sec. II. In this theory, the Hall constant is given as the sum of its infinite frequency limit (R_H^∞) and a memory-function contribution. The former term was considered by Shastry, Shraiman, and Singh.[3] Our emphasis is on the memory-function term which represents the deviation of the Hall constant from R_H^∞ for finite frequencies and thus cannot be neglected when considering the case of zero frequency. One advantage of our representation of the Hall constant is that we may dodge the issue of coping with a quotient of conductivities as opposed to the usual approaches. This is why the Hall constant at low frequencies becomes less sensitive to the detailed resonance structure of the conductivities. In Sec. III, this advantage is exploited for the range of weak to intermediate correlation strengths by calculating the memory function to second order in the Hubbard interaction and to first order in the magnetic field. Expansion with respect to the magnetic field leads to a decomposition of the memory function into two terms, namely a two-point and a three-point correlation function. Both contributions are evaluated exactly in infinite spatial dimensions. Our results indicate that the memory-function term is important. Only then, a precursor effect of the sign change of the Hall constant as a function of doping appears even in perturbation theory. Moreover, when extrapolating our results to U values of the order of twice the bare bandwidth W, we get most of the qualitative features observed in, e.g., $La_{2-x}Sr_xCuO_4$: the sign change with respect to doping and the decrease of the Hall constant up to unusually high temperatures, characteristic of most high-T_c compounds. However, the observed $1/\delta$ law of the Hall constant in the vicinity of half filling is not reproduced. It requires a description in the strong-correlation regime,[2] which will be the subject of Sec. IV. There, we first study the moments of the memory function in the limit $U\to\infty$. Thereby, the memory function is found to eliminate the high-energy scale set by the Hubbard repulsion U. This provides us with an explanation of the frequency dependence of the Hall constant in the crossover regime from $\omega\gg U$ to $W\ll\omega\ll U$. Furthermore, a simple analytical treatment of the Hall effect within the Hubbard I approximation is presented, the results of which turn out to be in full accord with that obtained by high-temperature expansions. Then, we reformulate the frequency-dependent Hall constant within the t-J model in order to address the low-frequency regime as well. The comparison to a representation of $R_H(\omega)$ in terms of two relaxation rates and effective masses introduced by Anderson[12] provides us with an interpretation of the additional relaxation rate τ_H in the language of the Mori theory and a phenomenological understanding of the anomalous frequency and temperature dependence of the Hall constant in high-T_c superconductors. Finally, we explain how the emerging picture may be put onto the basis of a microscopic calculation. In this context, we reduce the problem of calculating the memory function in the t-J model to the much easier one of finding the first few moments of the ordinary current-current correlation functions. Finally, in Sec. V, we summarize our main results.

II. THEORETICAL FRAMEWORK

A. Single-band Hubbard model

The single-band Hubbard model on a d-dimensional hypercubic lattice in a magnetic field reads

$$\hat{H}=\hat{T}+\hat{V}\ , \tag{1}$$

$$\hat{T}=-t\sum_{\langle ij\rangle\sigma}P_{ij}c_{i\sigma}^{+}c_{j\sigma}\ , \tag{2}$$

$$\hat{V}=U\sum_i\hat{n}_{i\uparrow}\hat{n}_{i\downarrow}\ , \tag{3}$$

where the sum in the hopping term $\hat{T}$ is restricted to nearest neighbors and $\hat{V}$ is the Hubbard repulsion. The Peierls phase factor $P_{ij}=\exp(ie\int_j^i\vec{A}(t,\vec{r})d\vec{r})$ guarantees the gauge invariance[13] and the sign of the charge e is chosen to be negative. Since only nearest-neighbor hops are taken into account, we may approximate

$$P_{ij}\simeq e^{ie\vec{A}(\vec{R}_j)(\vec{R}_i-\vec{R}_j)}\ , \tag{4}$$

where $\vec{R}_i$ denotes the lattice vector to site i. The vector potential decomposes into two terms describing the electric and magnetic field, respectively:

$$\vec{A}(t,\vec{r}\,)=\vec{A}^{\rm el}(t)+\vec{A}^{\rm mag}(\vec{r}\,)\ , \tag{5}$$

$$\vec{E}(t)=-\frac{\partial}{\partial t}\vec{A}^{\rm el}(t)\ , \tag{6}$$

$$\vec{H}=\mathrm{rot}\,\vec{A}^{\rm mag}(\vec{r}\,)\ . \tag{7}$$

In linear-response theory with respect to the electric field, the latter appears only in the definition of the current operator. More precisely, the current operator is defined as the following functional derivative:

$$\hat{J}_\nu:=-\frac{1}{e}\frac{\delta\hat{H}(t)}{\delta A_\nu^{\rm el}(t)}\bigg|_{A^{\rm el}=0}\ . \tag{8}$$

The homogeneous magnetic field is chosen to point in the z direction and it is advantageous to fix the gauge from the very beginning according to the Landau choice

$$\vec{A}^{\rm mag}(\vec{R})=R_xH\hat{y}\ , \tag{9}$$

since then, translational symmetry is broken only in one dimension, namely the x direction. $\hat{y}$ is a primitive lattice vector. We need the current operator only up to first order in the magnetic field:

$$\hat{J}_\nu=\hat{J}_\nu^{(0)}+\delta\hat{J}_\nu\ , \tag{10}$$

$$\hat{J}_\nu^{(0)}=it\sum_{\vec{R},\vec{R}+\vec{\delta},\sigma}\delta_\nu\,c_\sigma^{+}(\vec{R}+\vec{\delta})c_\sigma(\vec{R}), \tag{11}$$

$$\delta\hat{J}_\nu=-et\sum_{\vec{R},\vec{R}+\vec{\delta},\sigma}\delta_\nu\,\vec{\delta}\vec{A}^{\rm mag}(\vec{R})c_\sigma^{+}(\vec{R}+\vec{\delta})c_\sigma(\vec{R}). \tag{12}$$

Here, $\vec{\delta}$ is a nearest-neighbor vector and the summation is over pairs of nearest neighbors. Note, however, that due to the gauge fixation (9), we cannot choose periodic boundary conditions in the x direction. Thus, if $\vec{\delta}$ points in the x direction, we have to carry out the sums in such a way that the components R_x and $R_x+\delta_x$ are simultaneously elements of

the set consisting of the x coordinates of all lattice sites, i.e., $\{R_x^{\min}, R_x^{\min}+1, \ldots, R_x^{\max}\}$. Here, it is assumed that the lattice has N_x sites in the x direction which implies $R_x^{\max} \equiv R_x^{\min} + N_x - 1$. Of course, observable quantities are not allowed to depend on the lattice location $R_x^{\min}$. The hopping term is expanded analogously, yielding

$$\hat{T} = \hat{T}^{(0)} + \delta\hat{T} \ , \tag{13}$$

$$\hat{T}^{(0)} = -t \sum_{\vec{R},\vec{R}+\vec{\delta},\sigma} c_\sigma^+(\vec{R}+\vec{\delta}) c_\sigma(\vec{R}), \tag{14}$$

$$\delta\hat{T} = -iet \sum_{\vec{R},\vec{R}+\vec{\delta},\sigma} \vec{\delta}\vec{A}^{\mathrm{mag}}(\vec{R}) c_\sigma^+(\vec{R}+\vec{\delta}) c_\sigma(\vec{R}) \ . \tag{15}$$

The term without magnetic field, Eq. (14), becomes diagonal in crystal momentum space with a band dispersion $\epsilon_{\vec{k}} = -2t\Sigma_{j=1}^{d} \cos k_j$.

B. Mori theory

In this subsection, the basics of Mori's memory-function formalism are reviewed briefly. For further details, see, e.g., Ref. 14. The best known application of Mori theory is the description of many-particle systems in the hydrodynamic regime.[15] There, one is only interested in the dynamics of the hydrodynamic variables. They are characterized by the fact that their transport is restricted by conservation laws or by broken symmetries. Thus, they are bound to vary on a time scale that is very slow in comparison to that of all the other degrees of freedom. Now, the Mori theory enables one to separate these two time scales: The equations of motion of the hydrodynamic variables take on the form of coupled integrodifferential equations. The corresponding integral kernels of these so-called Mori equations are memory functions in which the influence of all the other degrees of freedom is accumulated, hence the name ''memory function.'' In this context of hydrodynamics, the memory functions are rapidly varying functions, whose effect may be simulated by damping constants. Then, the Mori equations take on a form analogous to that of the Langevin equation for a particle undergoing Brownian motion. However, the validity of the Mori equations is not restricted to the special set of hydrodynamic variables. In the simplest case, one sets up the Mori theory for those observables that constitute the correlation functions one is interested in. This leads to representations of the unknown correlation functions in terms of memory functions in which all analytic properties are fulfilled by construction. On the other hand, it may be difficult to find an approximate expression for a given memory function.

1. Basic notions

The *Liouville space* $\mathcal{L}$ is defined as the linear vector space over the field of complex numbers whose elements are the linear operators in the familiar Hilbert space of quantum mechanics, and where the usual operations like scalar multiplication, etc., hold. In this Liouville space exist linear operators that are called *superoperators* to distinguish them from the usual ones. (Henceforth, normal operators are denoted with a hat, superoperators not.) The most important superoperator is the *Liouville operator* L, which maps a given operator onto its commutator with the Hamiltonian:

$$L\hat{A} = [\hat{H}, \hat{A}] \ . \tag{16}$$

Another important class of superoperators are *superprojectors*. However, their definition implies a scalar product in $\mathcal{L}$. In the context of response functions, the most convenient scalar product turns out to be the so-called *Mori product*

$$(\hat{A}|\hat{B}) := \frac{1}{\beta}\int_0^\beta d\tau \, \langle \ e^{\tau L}\hat{A}^+ \cdot \hat{B} \ \rangle \ , \tag{17}$$

where $\langle \ldots \rangle$ denotes the thermal average and β is the inverse temperature. On the basis of this scalar product, we may now speak of adjoint superoperators S and S^+, and thus of unitary and Hermitian ones in the usual sense. The projector P that projects onto the subspace of $\mathcal{L}$ spanned by linearly independent elements $|\hat{G}_i)$, reads

$$P = \sum_{ij} |\hat{G}_i) g_{ij} (\hat{G}_j|, \tag{18}$$

where the metric g_{ij} is the inverse of the matrix $(\hat{G}_i|\hat{G}_j)$, i.e., $\Sigma_k \, g_{ik}(\hat{G}_k|\hat{G}_j) = \delta_{ij}$. In fact, this implies the idempotence property $P^2 = P$. Finally, the definition of the Mori product implies the validity of the so-called Kubo identity

$$\beta(\hat{A}|L|\hat{B}) = \langle [\hat{A}^+, \hat{B}] \rangle \ , \tag{19}$$

which will play an important role.

2. Memory-function approach to the Hall constant

From Eq. (19) follows a representation for the current-current correlation function $\langle\langle \hat{J}_\nu ; \hat{J}_\mu \rangle\rangle_z$, defined as the Laplace transform of $-i\langle [e^{iLt}\hat{J}_\nu, \hat{J}_\mu] \rangle$:

$$\langle\langle \hat{J}_\nu ; \hat{J}_\mu \rangle\rangle_z = -\beta \left(\hat{J}_\mu \left| \frac{L}{z+L} \right| \hat{J}_\nu \right) \equiv -\chi_{\mu\nu}(z) \ . \tag{20}$$

Here, z is a complex frequency, which ultimately has to be specialized to $\omega + i0^+$. For formal manipulations, however, it is more convenient to deal with the complex frequency z rather than with ω. The last expression has to be inserted into the Kubo formula for the conductivity tensor,

$$\sigma_{\nu\mu}(z) = \frac{ie^2}{Nz} \{ \langle \hat{\tau}_{\nu\mu} \rangle + \langle\langle \hat{J}_\nu ; \hat{J}_\mu \rangle\rangle_z \} \ , \tag{21}$$

where N is the total number of lattice sites and $\langle \hat{\tau}_{\nu\mu} \rangle$ arises from the equilibrium part of the current and is defined as the second functional derivative of the Hamiltonian with respect to the external electric field:

$$\hat{\tau}_{\nu\mu} := \frac{1}{e^2} \frac{\delta^2 \hat{H}(t)}{\delta A_\nu^{\mathrm{el}}(t) \, \delta A_\mu^{\mathrm{el}}(t)} \bigg|_{A^{\mathrm{el}}=0} \ . \tag{22}$$

In the Hubbard model (1), its expectation value is given as $\langle \hat{\tau}_{\nu\mu} \rangle = \delta_{\nu\mu} 2t \Sigma_{\vec{k}\sigma} \cos k_x \langle \hat{n}_{\vec{k}\sigma} \rangle$, i.e., as the average kinetic energy per dimension. Using the fact $\lim_{z\to 0} z\sigma_{\nu\mu}(z) = 0$ which

holds for a metal in the normal state, we show that $\langle \hat{\tau}_{\nu\mu} \rangle$ also equals the static susceptibility χ^0, defined through $\chi_{\mu\nu}(z=0) \equiv \delta_{\mu\nu}\, \chi^0$:

$$\chi^0 = \beta(\hat{J}_x | \hat{J}_x) = \langle \hat{\tau}_{xx} \rangle = -\frac{1}{d} \langle \hat{T} \rangle \quad . \tag{23}$$

Thus, the conductivity tensor may be written as

$$\sigma_{\nu\mu}(z) = \frac{e^2}{N} \beta \left(\hat{J}_\mu \left| \frac{i}{z+L} \right| \hat{J}_\nu \right) \equiv \frac{e^2}{N} C_{\mu\nu}(z) \ . \tag{24}$$

In order to represent the relaxation functions $C_{\mu\nu}(z)$ in terms of memory functions, we introduce the superprojector P that projects onto the subspace of $\mathcal{L}$ spanned by the current operators $\hat{J}_x$ and $\hat{J}_y$:

$$P = \frac{\beta}{\chi^0} \sum_{\nu=x,y} |\hat{J}_\nu)(\hat{J}_\nu| \ , \tag{25}$$

and the complementary superprojector $Q = 1 - P$. By making use of the operator identity $1/(a+b) = 1/a - (1/a) b [1/(a+b)]$ with $a \equiv z + LQ$ and $b \equiv LP$, we find

$$C_{\mu\nu}(z) = \frac{i}{z} \chi^0 \delta_{\mu\nu} - \frac{1}{z} R_{\mu\alpha}(z) C_{\alpha\nu}(z) \ , \tag{26}$$

$$R_{\mu\nu}(z) \equiv \frac{\beta}{\chi^0} \left(\hat{J}_\mu \left| \frac{z}{z+LQ} L \right| \hat{J}_\nu \right) \tag{27}$$

$$\equiv \Omega_{\mu\nu} + i M_{\mu\nu}(z) \ . \tag{28}$$

The terms in the last equation are the frequency and the memory matrix, respectively,

$$\Omega_{\mu\nu} \equiv \frac{1}{\chi^0} \langle [\hat{J}_\mu, \hat{J}_\nu] \rangle \quad , \tag{29}$$

$$M_{\mu\nu}(z) \equiv \frac{\beta}{\chi^0} \left(QL\hat{J}_\mu \left| \frac{i}{z+QLQ} \right| QL\hat{J}_\nu \right) \ . \tag{30}$$

The memory functions have the structure of relaxation functions for the so-called residual forces

$$\hat{f}_\nu = iQL\hat{J}_\nu , \tag{31}$$

whose dynamics is governed by the projected Liouville operator QLQ rather than L.[14] Thus, these forces may vary on a time scale that is different from that of the current operators $\hat{J}_\nu$. In Sec. IV B 1, we shall identify these two time scales with the relaxation rates of the holon and spinon degrees of freedom in Anderson's tomographic Luttinger liquid theory.[12] Solving Eq. (26) for the matrix $\mathbf{C}(z)$ leads to

$$\mathbf{C}(z) = i\chi^0 [z\mathbf{1} + \mathbf{\Omega} + i\mathbf{M}(z)]^{-1} \ . \tag{32}$$

Together with Eq. (24), this demonstrates that the Mori theory is heading directly for the resistivity tensor. Therefore, the desired representation for the dynamical Hall constant can be read off from the last equation:

$$R_H(z) = \frac{N}{ie^2\chi^0} \lim_{H\to 0} \frac{\Omega_{xy} + iM_{xy}(z)}{H} \quad . \tag{33}$$

Since the memory-function term will be shown to vanish in the high-frequency limit as $1/z^2$, the first term represents the high-frequency limit of the Hall constant considered by Shastry *et al.*:[3]

$$R_H^\infty = \frac{N}{ie^2\chi^0} \lim_{H\to 0} \frac{\Omega_{xy}}{H} \quad . \tag{34}$$

Moreover, Ω_{xy} is the generalization of the cyclotron frequency to the lattice case. Therefore, within a Boltzmann equation approach, only the term (34) is considered. The goal of the subsequent sections is to investigate the memory-function term $M(z) \equiv M_{xy}(z)$ for finite frequencies.

Before proceeding, we consider unperturbed Bloch electrons, described by the Hamiltonian (13). The fluctuating forces (31) contain the commutator of the current operator with the Hamiltonian. This commutator is of first order in the magnetic field, since the current of Bloch electrons is conserved in the absence of a magnetic field. Hence the memory function $M(z)$ is of second order in the magnetic field and, therefore, does not contribute to the Hall constant. This demonstrates that the Hall constant of Bloch electrons is frequency independent and given by Eq. (34). Note also that conductivities are finite in the limit $\alpha \to 0$ only if there are inelastic processes that can degrade the total crystal momentum. Although this condition is not satisfied in the case of unperturbed Bloch electrons, their Hall constant can be calculated for *all* frequencies.

3. Analytic properties

The analytic properties of $M(z)$ in Eq. (33) may all be derived on the basis of Eq. (30). An alternative procedure is to solve Eq. (32) for $\mathbf{M}(z)$ and go back to the analytic properties of the current susceptibilities $\chi_{\mu\nu}(z)$, cf. Eq. (20). $M(z)$ reads in terms of the susceptibilities $\chi_{\mu\nu}(z)$:

$$iM(z) = \frac{z\chi^0 \chi_{xy}(z)}{[\chi^0 - \chi_{xx}(z)]^2} - \frac{\langle [\hat{J}_x, \hat{J}_y] \rangle}{\chi^0} \quad . \tag{35}$$

From time-reversal invariance, homogeneity of time and the fact that the current operators are Hermitian, we may deduce the following symmetry properties:[15]

$$\chi_{xx}(-z) = \chi_{xx}(z) \ , \tag{36}$$

$$\chi_{xx}^*(z) = \chi_{xx}(z^*) \ , \tag{37}$$

$$\chi_{xy}(-z) = -\chi_{xy}(z) \ , \tag{38}$$

$$\chi_{xy}^*(z) = -\chi_{xy}(z^*) \ . \tag{39}$$

Together with Eq. (35), this implies

$$M(-z) = M(z) \ , \tag{40}$$

$$M^*(z) = M(z^*) \ . \tag{41}$$

$M(z)$ can be represented as a spectral integral

$$M(z) = \int \frac{d\omega}{\pi} \frac{M''(\omega)}{\omega - z} \ , \tag{42}$$

where the spectral function $M''(\omega)$ is given by the discontinuity across the real axis:

$$M(\omega \pm i0^+) = M'(\omega) \pm iM''(\omega) \ . \tag{43}$$

From the analytic properties (40) and (41), it follows that $M'(\omega)$ and $M''(\omega)$ are real functions satisfying

$$M'(-\omega) = M'(\omega) \ , \tag{44}$$

$$M''(-\omega) = -M''(\omega) \ . \tag{45}$$

Thus, two further conclusions can be drawn: Firstly, only even powers in $1/z$ contribute to the high-frequency expansion of $M(z)$. And secondly, the quotient $M''(\omega)/\omega$ must be integrable around $\omega = 0$,

$$\int_{-\infty}^{\infty} d\omega \ M''(\omega)/\omega < \infty, \tag{46}$$

which can be seen from the fact that the dc-Hall constant contains this integral. Note, that we need not understand this expression as a Principal value integral due to the fact that the integrand is even.

III. PERTURBATION THEORY

Despite many interesting works on the normal-state Hall effect of high-T_c superconductors, a calculation that incorporates all the complicated many-body correlations within a microscopic model is still lacking. The following treatment of the Hall constant closes this gap at least in the perturbation-theoretical regime. On the other hand, the relevant parameter regime is believed to be the strong-correlation limit rather than the weak one. However, it turns out that the final expression may well describe the observed dependences on temperature and on doping at least qualitatively, if we allow U to be extrapolated to values of the order of the bare bandwidth W. Thus, a precursor effect of the anomalous dependences clearly shows up even in the regime of weak correlations.

A. Approximation

The perturbation-theoretical treatment of the Hall constant is by no means straightforward. As is well known, the evaluation of response functions like $\chi_{\mu\nu}(z)$ of Eq. (20) by expansion in a small interaction parameter fails because, as an artifact of such an expansion, these functions become singular for small frequencies z. This difficulty was resolved by Götze and Wölfle[16] some time ago by means of a memory-function approach. They calculated the memory function perturbatively, which, at first, is valid only at high enough frequencies. It turns out, however, that their expression for the memory function depends only smoothly on frequency below a certain frequency scale and tends to a constant in the limit $\omega \to 0$. Furthermore, in their approximation scheme the correct resonance structure of the studied response functions is inherently built in. Thus, their results could be used in the whole frequency regime including the hydrodynamic one. However, we cannot carry over their analysis straightforwardly to the present problem, because otherwise, we would encounter a spurious singularity in the limit that is of most interest, namely the limit $\omega \to 0$.

In this subsection, we identify the precondition which is necessary to obtain regular expressions in this limit and that was fulfilled trivially in the applications of Ref. 16 but is not in our case. Since this condition does not affect the correct description of the local interaction U, we may take it as an approximation. By using Mori's formalism, we shall see that once this condition is assumed to be satisfied no further approximations have to be made. This last point cannot be seen in the more intuitive introduction of the memory-function concept as given in Ref. 16 and shows that the extrapolation to low frequencies therein is exact.

Perturbation theory is based on the following decomposition of the Liouville operator:

$$L = L_0 + L_1, \tag{47}$$

where L_0 and L_1 are assigned to the hopping and interaction term of the Hubbard Hamiltonian (1), respectively. The perturbation-theoretical regime is given by the condition $U \ll W$, where W is the width of the bare band and thus represents the characteristic energy scale introduced by L_0. The precondition to obtain a regular expression for the memory function $M(z)$ for all frequencies to leading order in U is that the relevant operators $\hat{J}_x$ and $\hat{J}_y$ span a subspace of $\mathcal{L}$ that is invariant with respect to actions of L_0.[14] If this condition were satisfied in our case, it would take on the form

$$L_0 \hat{J}_\nu = [\hat{T}, \hat{J}_\nu] = \hat{J}_\mu \Omega^0_{\mu\nu}, \tag{48}$$

where $\nu, \mu = x, y$ and summation over repeated indices is implied. This can be checked by inserting these equations into $(\hat{J}_\lambda | \ldots)_0$ and comparing the result with the definition (29). $(\ldots | \ldots)_0$ is the Mori product with respect to L_0. Since only terms of the first order in the magnetic field H are to be kept [cf. Eq. (33)], we may take the current operator on the right-hand side (rhs) of Eq. (48) at $H = 0$. Henceforth, bracketed superscripts or subscripts refer to the magnetic field and unbracketed ones to the decomposition (47). Unfortunately, the conditions (48) are not satisfied in the Hubbard model. Instead, we derive with the help of Eqs. (10)–(12) and (13)–(15) (see Appendix A):

$$[\hat{T}, \hat{J}_x] = \frac{\sum_{\vec{k}\sigma} \cos k_x \sin k_y \, \hat{n}_{\vec{k}\sigma}}{\sum_{\vec{k}\sigma} \cos k_x \cos k_y \, n^0_{\vec{k}\sigma}} \ \langle [\hat{J}_y, \hat{J}_x] \rangle_0 \ , \tag{49}$$

which should be equal to

$$\frac{\sum_{\vec{k}\sigma} \sin k_y \, \hat{n}_{\vec{k}\sigma}}{\sum_{\vec{k}\sigma} \cos k_y \, n^0_{\vec{k}\sigma}} \ \langle [\hat{J}_y, \hat{J}_x] \rangle_0 = \hat{J}^{(0)}_y \Omega^0_{yx} \ . \tag{50}$$

This is obviously not the case. Similarly, we find

$$[\hat{T},\hat{J}_y] = \frac{\sum_{\vec{k}\sigma} \sin k_x \cos k_y \, \hat{n}_{\vec{k}\sigma}}{\sum_{\vec{k}\sigma} \cos k_x \cos k_y \, n^0_{\vec{k}\sigma}} \langle [\hat{J}_x,\hat{J}_y]\rangle_0 \ , \qquad (51)$$

instead of

$$\frac{\sum_{\vec{k}\sigma} \sin k_x \, \hat{n}_{\vec{k}\sigma}}{\sum_{\vec{k}\sigma} \cos k_x \, n^0_{\vec{k}\sigma}} \langle [\hat{J}_x,\hat{J}_y]\rangle_0 = \hat{J}_x^{(0)} \Omega^0_{xy} \ . \qquad (52)$$

However, the conditions (48) become exact in the continuum limit or in the limit of small band fillings. This is seen if we take explicitly into account the lattice spacing a in the arguments of the trigonometric functions which we tacitly have set equal to 1. Then we may expand $\cos k_\nu a \simeq 1$ and $\sin k_\nu a \simeq k_\nu a$ which proves the statement immediately. Thus, the violation of the conditions (48) on the lattice reflects its reduced symmetry in comparison with free space. Since the conditions (48) are properties of the *free* model, we may assume their approximate validity without taking the risk of not describing the local interactions (3) correctly.

Before proceeding, we show how the conditions (48) appear within the formalism outlined in Ref. 16. We expand Eq. (35) in the frequency regime, where the expression $|\chi_{xx}(z)/\chi^0|$ is very small, i.e., for high enough frequencies and use a couple of times equations of motion for correlation functions $\langle\langle \hat{A};\hat{B}\rangle\rangle_z$. Thus we may show that $M(z)$ can be represented as follows [cf. Eq. (57)]:

$$i\chi^0 M(z) \simeq - \frac{\langle\langle \hat{K}_x;\hat{K}_y\rangle\rangle^0_z}{z} + R(z) \ . \qquad (53)$$

The first term will be investigated in the next subsection and turns out to be regular for all frequencies; $R(z)$ can be written as

$$R(z) = \langle\langle \hat{J}_x;[\hat{T},\hat{J}_y]\rangle\rangle_z - \langle\langle [\hat{T},\hat{J}_x];\hat{J}_y\rangle\rangle_z + 2\Omega^0_{xy}\chi_{xx}(z)$$
$$= \frac{2\langle [\hat{J}_x,\hat{J}_y]\rangle_0}{\chi^0} \frac{\phi_{xx}(z)-\phi_{xx}(0)}{z^2} \ , \qquad (54)$$

where $\phi_{xx}(z) \equiv \langle\langle \hat{K}_x;\hat{K}_x\rangle\rangle^0_z$. Calculating the function $\phi_{xx}(z)$ by following the lines outlined in the next subsection, we may prove that $R(z)$ is indeed divergent in the limit $z \to 0$, which, however, is an artifact of perturbation theory. The first representation of $R(z)$ in the last set of equations shows that the condition (48) implies $R(z)$ to vanish identically, if we take into account the symmetry properties $\Omega^0_{xy} = -\Omega^0_{yx}$ and $\chi_{xx}(z) = \chi_{yy}(z)$.

B. Reduction to ordinary correlation functions

We are interested in the memory function appearing in Eq. (33), whose Laplace transform is given according to Eq. (30) as

$$M(t) = \frac{\beta}{\chi^0} (QL\hat{J}_x | e^{iQLQt} | QL\hat{J}_y) \ . \qquad (55)$$

Due to the approximation (48), the free part L_0 of the Liouville operator does not contribute to the operator $QL|\hat{J}_\nu)$. Hence, to leading order in the interaction strength U, we obtain

$$M(t) = \frac{\beta}{\chi^0} (Q_0 L_1 \hat{J}_x | e^{iQ_0 L_0 Q_0 t} | Q_0 L_1 \hat{J}_y)_0 \ . \qquad (56)$$

Since Q_0 commutes with L_0 and because of the idempotence of Q_0,[14] we may free ourselves of all superprojectors Q_0 with the exception of one, say, that within the ''ket'' $|Q_0 L_1 \hat{J}_y)$. However, even this last appearance of Q_0 may be omitted, since its part P_0 leads to a term proportional to the following first-order expression of the frequency matrix:[14] $\Omega^1_{\nu\mu} = g^0_{\nu\lambda} (\hat{J}_\lambda | L_1 | \hat{J}_\mu)_0$. Here summation over equal indices is implied. However, the frequency matrix is easily traced back to $n_{\vec{k}\sigma} = \langle c^+_{\vec{k}\sigma} c_{\vec{k}\sigma}\rangle$, whose first-order contribution vanishes. Thus, $\Omega^1_{\nu\mu}$ vanishes as stated and we arrive at $M(z) = (\beta/\chi^0)(\hat{K}_x | i/(z+L_0) | \hat{K}_y)_0$, where we have defined

$$\hat{K}_\nu \equiv [\hat{V},\hat{J}_\nu] \ . \qquad (57)$$

With the identity $z/(z+L_0) = 1 - L_0/(z+L_0)$ and the symmetry property $\langle\langle \hat{K}_x;\hat{K}_y\rangle\rangle^0_{-z} = -\langle\langle \hat{K}_x;\hat{K}_y\rangle\rangle^0_z$, which may be traced back to Eq. (38) by means of two equations of motion, we eventually arrive at

$$i\chi^0 M(z) = - \frac{\langle\langle \hat{K}_x;\hat{K}_y\rangle\rangle^0_z}{z} \ . \qquad (58)$$

Now, we must evaluate this correlation function for the free tight-binding model (13) to leading first order in the magnetic field. In order to derive explicit expressions for the operators (57), we introduce the following combination of Bloch operators:

$$\hat{A}^\sigma_{\vec{k}_1,\vec{k}_2|\vec{k}|\vec{q}} \equiv c^+_{\vec{k}_1\sigma} c_{\vec{k}_2\sigma} c^+_{\vec{k}-\vec{q}|-\sigma} c_{\vec{k}|-\sigma} \ . \qquad (59)$$

This is the basic building block of the operators $\hat{K}_\nu$. To see this, we insert Eqs. (3) and (10)–(12) into the definition (57) and write the result in terms of Bloch operators. We find

$$\hat{K}_\nu = \hat{K}^{(0)}_\nu + \delta\hat{K}_\nu , \qquad (60)$$

$$\hat{K}^{(0)}_\nu = - \frac{U}{N} \sum_{\vec{k}_1\vec{k}_2\vec{k}\vec{q}\sigma} [B_\nu(\vec{k}_1,\vec{k}_2+\vec{q}\,) - B_\nu(\vec{k}_1-\vec{q},\vec{k}_2)] \hat{A}^\sigma_{\vec{k}_1,\vec{k}_2|\vec{k}|\vec{q}} \ , \qquad (61)$$

$$\delta\hat{K}_x = 0 \ , \qquad (62)$$

$$\delta\hat{K}_y = Het \frac{U}{N} \sum_{\vec{k}_1\vec{k}_2\vec{k}\vec{q}\sigma} [C(\vec{k}_1,\vec{k}_2+\vec{q}\,) - C(\vec{k}_1-\vec{q},\vec{k}_2)] \hat{A}^\sigma_{\vec{k}_1,\vec{k}_2|\vec{k}|\vec{q}} \ , \qquad (63)$$

where the matrices $B_\nu(\vec{k}_1,\vec{k}_2)$ and $C(\vec{k}_1,\vec{k}_2)$ are defined in Appendix A, cf. Eqs. (A2) and (A3). Since $\delta\hat{K}_x$ vanishes,

the expansion of the correlation function appearing in Eq. (58) to first order in the magnetic field reads

$$\langle\langle \hat{K}_x;\hat{K}_y\rangle\rangle_z^0 = C^{II}(z)+C^{III}(z)\ , \tag{64}$$

$$C^{II}(z)=\langle\langle \hat{K}_x^{(0)};\delta\hat{K}_y\rangle\rangle_z^{0(0)}, \tag{65}$$

$$C^{III}(z)=\langle\langle \hat{K}_x^{(0)};\hat{K}_y^{(0)}\rangle\rangle_z^{0(1)}. \tag{66}$$

Obviously, it is sufficient to calculate the correlation function consisting of operators (59) within the tight-binding model (13), however, to first order in the magnetic field. But first, we note that the functions (65) and (66) are two- and three-point correlation functions, respectively. This is explicitly seen within the Matsubara representation where the expansion of $\langle\langle \hat{K}_x;\hat{K}_y\rangle\rangle_z^0$ up to first order in the ''perturbation'' Eq. (15) yields

$$C^{II}(i\omega_m)=-\frac{1}{\beta}\int_0^\beta\int_0^\beta d\tau\, d\tau'\ \langle T_\tau\{\hat{K}_x^{(0)}(\tau)\ \delta\hat{K}_y(\tau')\}\rangle_0^{(0)} \times e^{i\omega_m(\tau-\tau')}\ , \tag{67}$$

$$C^{III}(i\omega_m)=\frac{1}{\beta}\int_0^\beta\int_0^\beta\int_0^\beta d\tau\, d\tau' d\tau''\ \langle T_\tau\{\hat{K}_x^{(0)}(\tau)\hat{K}_y^{(0)}(\tau') \times\delta\hat{T}(\tau'')\}\rangle_0^{(0)} e^{i\omega_m(\tau-\tau')}. \tag{68}$$

C. Expansion to first order in the magnetic field

As already mentioned, our next goal is to calculate the correlation function generated by the operators (59) up to first order in the magnetic field. This is accomplished by means of its equation of motion with respect to the tight-binding Hamiltonian (13):

$$\begin{aligned}(z+\epsilon_{\vec{k}-\vec{q}}-\epsilon_{\vec{k}}+\epsilon_{\vec{k}_1}-\epsilon_{\vec{k}_2})\langle\langle \hat{A}^{\sigma}_{\vec{k}_1,\vec{k}_2|\vec{k}|\vec{q}};\ \hat{A}^{\sigma'}_{\vec{k}_1',\vec{k}_2'|\vec{k}'|\vec{q}'}\rangle\rangle_z \\ =\langle[\hat{A}^{\sigma}_{\vec{k}_1,\vec{k}_2|\vec{k}|\vec{q}},\ \hat{A}^{\sigma'}_{\vec{k}_1',\vec{k}_2'|\vec{k}'|\vec{q}'}]\rangle \\ -\langle\langle[\delta\hat{T},\hat{A}^{\sigma}_{\vec{k}_1,\vec{k}_2|\vec{k}|\vec{q}}];\hat{A}^{\sigma'}_{\vec{k}_1',\vec{k}_2'|\vec{k}'|\vec{q}'}\rangle\rangle_z^{(0)}\ .\end{aligned} \tag{69}$$

Here and in the following, the superscript 0 is omitted. The expansion of the expectation value on the rhs with respect to the magnetic field is standard[17] and yields

$$\langle[\hat{A}^{\sigma}_{\vec{k}_1,\vec{k}_2|\vec{k}|\vec{q}},\hat{A}^{\sigma'}_{\vec{k}_1',\vec{k}_2'|\vec{k}'|\vec{q}'}]\rangle=\langle[\hat{A}^{\sigma}_{\vec{k}_1,\vec{k}_2|\vec{k}|\vec{q}},\hat{A}^{\sigma'}_{\vec{k}_1',\vec{k}_2'|\vec{k}'|\vec{q}'}]\rangle^{(0)} -\langle\hat{v}[\hat{A}^{\sigma}_{\vec{k}_1,\vec{k}_2|\vec{k}|\vec{q}},\hat{A}^{\sigma'}_{\vec{k}_1',\vec{k}_2'|\vec{k}'|\vec{q}'}]\rangle^{(0)}\ , \tag{70}$$

where $\hat{v}$ arises from the expansion of the S-matrix related to the ''perturbation'' (15) and is therefore given by

$$\hat{v}=\int_0^\beta d\tau\ \ e^{\tau(\hat{T}^{(0)}-\mu\hat{N})}\delta\hat{T}e^{-\tau(\hat{T}^{(0)}-\mu\hat{N})}\ . \tag{71}$$

With the representation of $\delta\hat{T}$ in terms of Bloch operators,

$$\delta\hat{T}=-ietH\sum_{\vec{k}_1\vec{k}_2\sigma}D(\vec{k}_1,\vec{k}_2)c^+_{\vec{k}_1\sigma}c_{\vec{k}_2\sigma}\ , \tag{72}$$

where the matrix $D(\vec{k}_1,\vec{k}_2)$ is also defined and further evaluated in Appendix A [cf. Eq. (A4)], we find more explicitly

$$\hat{v}=-ietH\sum_{\vec{k}_1\vec{k}_2\sigma}D(\vec{k}_1,\vec{k}_2)\frac{e^{\beta(\epsilon_{\vec{k}_1}-\epsilon_{\vec{k}_2})}-1}{\epsilon_{\vec{k}_1}-\epsilon_{\vec{k}_2}}c^+_{\vec{k}_1\sigma}c_{\vec{k}_2\sigma}\ . \tag{73}$$

Inserting the expansion (70) into Eq. (69), we obtain the following zeroth and first-order terms of the correlation function to be determined:

$$\langle\langle \hat{A}^{\sigma}_{\vec{k}_1,\vec{k}_2|\vec{k}|\vec{q}};\hat{A}^{\sigma'}_{\vec{k}_1',\vec{k}_2'|\vec{k}'|\vec{q}'}\rangle\rangle_z^{(0)}=\frac{\langle[\hat{A}^{\sigma}_{\vec{k}_1,\vec{k}_2|\vec{k}|\vec{q}},\hat{A}^{\sigma'}_{\vec{k}_1',\vec{k}_2'|\vec{k}'|\vec{q}'}]\rangle^{(0)}}{z+\epsilon_{\vec{k}-\vec{q}}-\epsilon_{\vec{k}}+\epsilon_{\vec{k}_1}-\epsilon_{\vec{k}_2}}, \tag{74}$$

$$\begin{aligned}\langle\langle \hat{A}^{\sigma}_{\vec{k}_1,\vec{k}_2|\vec{k}|\vec{q}};\hat{A}^{\sigma'}_{\vec{k}_1',\vec{k}_2'|\vec{k}'|\vec{q}'}\rangle\rangle_z^{(1)} \\ =-\frac{\langle\hat{v}\ \ [\hat{A}^{\sigma}_{\vec{k}_1,\vec{k}_2|\vec{k}|\vec{q}},\hat{A}^{\sigma'}_{\vec{k}_1',\vec{k}_2'|\vec{k}'|\vec{q}'}]\rangle^{(0)}}{z+\epsilon_{\vec{k}-\vec{q}}-\epsilon_{\vec{k}}+\epsilon_{\vec{k}_1}-\epsilon_{\vec{k}_2}} \\ -\frac{\langle\langle[\delta\hat{T},\hat{A}^{\sigma}_{\vec{k}_1,\vec{k}_2|\vec{k}|\vec{q}}]\ ;\ \hat{A}^{\sigma'}_{\vec{k}_1',\vec{k}_2'|\vec{k}'|\vec{q}'}\rangle\rangle_z^{(0)}}{z+\epsilon_{\vec{k}-\vec{q}}-\epsilon_{\vec{k}}+\epsilon_{\vec{k}_1}-\epsilon_{\vec{k}_2}}\ .\end{aligned} \tag{75}$$

The second term on the rhs of Eq. (75) still contains a correlation function. Fortunately, this function is related to the Hamiltonian (14) without magnetic field thus being directly reducible to expectation values by means of its equation of motion:

$$\langle\langle[\delta\hat{T},\hat{A}^{\sigma}_{\vec{k}_1,\vec{k}_2|\vec{k}|\vec{q}}];\hat{A}^{\sigma'}_{\vec{k}_1',\vec{k}_2'|\vec{k}'|\vec{q}'}\rangle\rangle_z^{(0)} =\frac{\langle[[\delta\hat{T},\hat{A}^{\sigma}_{\vec{k}_1,\vec{k}_2|\vec{k}|\vec{q}}],\hat{A}^{\sigma'}_{\vec{k}_1',\vec{k}_2'|\vec{k}'|\vec{q}'}]\rangle_z^{(0)}}{z-\epsilon_{\vec{k}'-\vec{q}'}+\epsilon_{\vec{k}'}-\epsilon_{\vec{k}_1'}+\epsilon_{\vec{k}_2'}}. \tag{76}$$

In summary, the problem of calculating the memory function (58) to leading order in the magnetic field has been reduced to the calculation of expectation values within the unperturbed tight-binding model without magnetic field: The relevant information is contained in Eqs. (61), (63)–(66), and (74)–(76). The rather cumbersome calculations are roughly sketched out in Appendix B. We write the memory-function contribution to the Hall constant [cf. Eq. (33)] as follows:

$$\delta R_H(z)=\frac{1}{e}\left(\frac{U}{2ta_n^0}\right)^2[m^{II}(z)+m^{III}(z)]\ , \tag{77}$$

where a_n is the amplitude of a nearest-neighbor hop and is related to the static susceptibility Eq. (23) via $\chi^0=4tNa_n$. This, in turn, implies

$$a_n=\frac{1}{2N}\sum_{k\sigma}\cos k_x\, n_{\vec{k}\sigma}. \tag{78}$$

$m^{II}(z)$ and $m^{III}(z)$ arise from the two- and three-point correlation functions, respectively, and are represented with regard to the further strategy as energy integrals:

$$m^{II}(z)=-\frac{t^2}{d}\int d\epsilon_1\int d\epsilon_2\int d\epsilon_1'\int d\epsilon_2'\; I(z|\epsilon_1,\epsilon_2|\epsilon_1',\epsilon_2')L^{II}(\epsilon_1,\epsilon_2|\epsilon_1',\epsilon_2') \quad , \tag{79}$$

$$m^{III}(z)=\frac{t^3}{\sqrt{d}}[Q(z)+Q(-z)] \; , \tag{80}$$

$$Q(z)=\int d\epsilon\int d\epsilon_1\int d\epsilon_2\int d\epsilon_1'\int d\epsilon_2'\;\frac{I(z|\epsilon,\epsilon_2|\epsilon_1',\epsilon_2')-I(z|\epsilon_1,\epsilon_2|\epsilon_1',\epsilon_2')}{\epsilon-\epsilon_1}L^{III}(\epsilon|\epsilon_1,\epsilon_2|\epsilon_1',\epsilon_2') \quad . \tag{81}$$

The integrands feature the following abbreviations:

$$I(z|\epsilon_1,\epsilon_2|\epsilon_1',\epsilon_2')\equiv\frac{f(\epsilon_1)f(\epsilon_2)[1-f(\epsilon_1')][1-f(\epsilon_2')]-[1-f(\epsilon_1)][1-f(\epsilon_2)]f(\epsilon_1')f(\epsilon_2')}{(\epsilon_1+\epsilon_2-\epsilon_1'-\epsilon_2')(z+\epsilon_1+\epsilon_2-\epsilon_1'-\epsilon_2')} \quad , \tag{82}$$

$$\begin{aligned}\frac{L^{II}(\epsilon_1,\epsilon_2|\epsilon_1',\epsilon_2')}{d}\equiv\Big\langle\;&\delta(\epsilon_1-\epsilon_{\vec{k}_1})\,\delta(\epsilon_2-\epsilon_{\vec{k}_2})\,\delta(\epsilon_1'-\epsilon_{\vec{k}_1'})\,\delta(\epsilon_2'-\epsilon_{\vec{k}_2'})\Big\{\cos k_{1x}+\cos k_{1x}'-[\sin k_{1x}-\sin k_{1x}']\\&\times\mathcal{P}\cot\left(\frac{k_{1x}+k_{2x}-k_{1x}'-k_{2x}'}{2}\right)\Big\}\{\cos k_{1y}+\cos k_{2y}-\cos k_{1y}'-\cos k_{2y}'\}\\&\times 2\pi\delta(k_{1y}+k_{2y}-k_{1y}'-k_{2y}')\Big\rangle_{\vec{k}_1\vec{k}_2\vec{k}_1'\vec{k}_2'},\end{aligned} \tag{83}$$

$$\begin{aligned}\frac{L^{III}(\epsilon|\epsilon_1,\epsilon_2|\epsilon_1',\epsilon_2')}{-2\sqrt{d}}\equiv\Big\langle\;&\delta(\epsilon-\epsilon_{\vec{k}_1'+\vec{k}_2'-\vec{k}_2})\,\delta(\epsilon_1-\epsilon_{\vec{k}_1})\,\delta(\epsilon_2-\epsilon_{\vec{k}_2})\,\delta(\epsilon_1'-\epsilon_{\vec{k}_1'})\,\delta(\epsilon_2'-\epsilon_{\vec{k}_2'})\Big\{\cos k_{1x}+\cos k_{2x}+\cos k_{1x}'+\cos k_{2x}'\\&-[\sin k_{1x}+\sin k_{2x}-\sin k_{1x}'-\sin k_{2x}']\;\mathcal{P}\cot\left(\frac{k_{1x}+k_{2x}-k_{1x}'-k_{2x}'}{2}\right)\Big\}\\&\times\{\sin k_{1y}+\sin k_{2y}-\sin k_{1y}'-\sin k_{2y}'\}\sin k_{1y}2\pi\delta(k_{1y}+k_{2y}-k_{1y}'-k_{2y}')\Big\rangle_{\vec{k}_1\vec{k}_2\vec{k}_1'\vec{k}_2'},\end{aligned} \tag{84}$$

and $f(\epsilon)\equiv 1/[\exp(\beta(\epsilon-\mu))+1]$ is the Fermi function. $\langle\cdots\rangle_{\vec{k}}$ denotes the average over the first Brillouin zone, i.e., $\int d^dk/(2\pi)^d(\cdots)$. Note, that the last two equations (83) and (84) reflect the gauge fixation (9): In the y direction, crystal momentum is conserved which is ensured by the δ functions while the x components of the Bloch vectors are coupled more complicatedly. In principle, we could do the momentum integrations numerically for a two-dimensional lattice and for given sets of external parameters temperature T, doping δ, and frequency ω. However, we prefer to carry on our analysis a little bit by invoking a limit pioneered by Metzner and Vollhardt in the context of strongly correlated electrons,[18] namely the limit of infinite spatial dimensions. In this limit, the momentum integrals decouple and we are left with energy integrals over smooth functions. This procedure will be discussed in the next subsection.

D. The limit of infinite lattice dimensions

We may question the relevance of this limit, since the important physics of the high-T_c superconductors is known to take place in Cu-O planes. Many authors have addressed this issue and much evidence has been revealed in favor of the relevance of this limiting procedure even for two-dimensional systems; see, e.g., Ref. 19. Instead of immersing ourselves in this debate, we take the following point of view: The main reasons behind the anomalous properties of the high-T_c materials seem to be, firstly, the strong electronic correlations and, secondly, the two-dimensionality of the relevant Cu-O planes. Taking the limit $d\to\infty$ helps us to sepa-

rate the impact of the correlations and to suppress effects of low-dimensionality like, e.g., van Hove singularities. In this sense, the limit $d\to\infty$ is interesting in itself.

For our problem, the most important aspect of the limit $d\to\infty$ is the following: For the Hubbard model to retain its nontrivial dynamics, the parameter t has to be scaled properly with d according to

$$2t=\frac{t^*}{\sqrt{d}} \tag{85}$$

(in this subsection, we set $t^*\equiv 1$). Only then does the Hubbard model capture simultaneously the itinerant and local aspects introduced by the hopping and interaction terms, respectively. On the other hand, we are tempted to conclude from the scaling (85) that any transport stops to be possible in $d=\infty$. In fact, a more thorough investigation shows that the longitudinal and the Hall conductivity are of order $1/d$ and $1/d^2$, respectively. But this, in turn, implies that the Hall constant remains finite in $d\to\infty$. In the following, all we need to know is how to calculate averages over Brillouin zones of the type Eqs. (83) and (84). The corresponding procedure is explained in Appendix C and enables us also to calculate simpler quantities as the density of states $D(\epsilon)$ of the band model (14), the nearest-neighbor hopping amplitude (78), and the amplitude of a hop diagonally across the unit cell, i.e.,

$$a_d=\frac{1}{2N}\sum_{\vec{k}\sigma}\cos k_x\cos k_y n_{\vec{k}\sigma}. \tag{86}$$

In the case of the amplitudes (78) and (86), the functions

$$A(\epsilon)\equiv\langle\cos k_x\ \delta(\epsilon-\epsilon_{\vec{k}})\rangle_{\vec{k}}=-\frac{\epsilon}{\sqrt{d}}D(\epsilon)\quad , \tag{87}$$

$$B(\epsilon)\equiv\langle\cos k_x\cos k_y\ \delta(\epsilon-\epsilon_{\vec{k}})\rangle_{\vec{k}}=\frac{1}{d}\left(\epsilon^2-\frac{1}{2}\right)D(\epsilon) \tag{88}$$

come into play. Essentially, they are Gaussians multiplied with the first and second Hermitian polynomial, respectively, since they are derivatives of the Gaussian density of states:

$$D(\epsilon)=\frac{1}{\sqrt{\pi}}\,e^{-\epsilon^2}\quad . \tag{89}$$

The functions (83) and (84) are found to be combinations of the functions (87) and (88) and may be written as

$$L^{II}(\epsilon_1,\epsilon_2|\epsilon_1',\epsilon_2')=D(\epsilon_1)D(\epsilon_2)D(\epsilon_1')D(\epsilon_2')\{\epsilon_1^2+\epsilon_1\epsilon_2+\epsilon_2\epsilon_1'-\epsilon_1'^2-\epsilon_1'\epsilon_2'-\epsilon_2'\epsilon_1\}\quad , \tag{90}$$

$$L^{III}(\epsilon|\epsilon_1,\epsilon_2|\epsilon_1',\epsilon_2')=D(\epsilon)D(\epsilon_1)D(\epsilon_2)D(\epsilon_1')D(\epsilon_2')\times\{-\epsilon+\epsilon_1+\epsilon_2+\epsilon_1'+\epsilon_2'\}\quad . \tag{91}$$

In order to handle the singularity of the Hall constant in the empty band limit correctly, we shall discuss the perturbation-theoretical result for the Hall constant normalized to its $U\to 0$ limit:

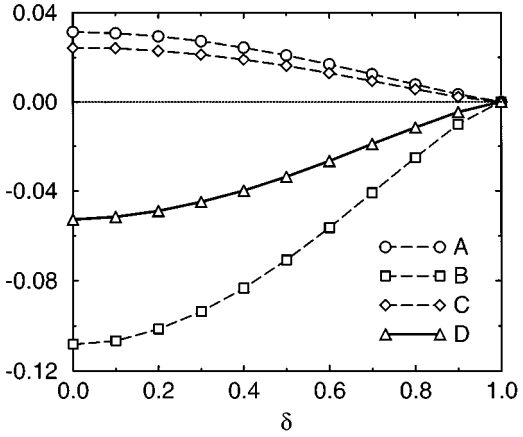

FIG. 1. The corrections of Eq. (92) at $T=0$. The curves A, B, C, and D represent the functions $K^{\infty}(\delta)$, $K^{II}(\delta)$, $K^{III}(\delta)$, and their sum, respectively.

$$\frac{R_H(z,U)}{R_{H0}}=1+U^2[K^{\infty}+K^{II}(z)+K^{III}(z)]\quad . \tag{92}$$

$K^{II}(z)$ and $K^{III}(z)$ arise from the functions (79) and (80), respectively, e.g., $K^{II}(z)=(2d/a_{d0})m^{II}(z)$. K^{∞} is the perturbation-theoretical contribution of the infinite frequency Hall constant (34). The latter may be written in terms of the amplitudes (78) and (86):

$$R_H^{\infty}=\frac{1}{e}\frac{2a_d}{(2a_n)^2}\quad . \tag{93}$$

This holds on account of the following relations, which may be proven by straightforward analysis:

$$\langle[\hat{J}_x,\hat{J}_y]\rangle=8iNet^2Ha_d, \tag{94}$$

$$\chi^0=4tNa_n. \tag{95}$$

Therefore, it is sufficient to calculate the density $n_{\vec{k}\sigma}$ to second order in U. The derivation is standard and will therefore not be given here. Similarly, the $U=0$ Hall constant is given by

$$R_{H0}=\frac{1}{e}\frac{2a_{d0}}{(2a_{n0})^2} \tag{96}$$

(the subscripts 0 indicate $U=0$ as above). Due to symmetries of the expression (91), the function (81) may be simplified by means of various redefinitions of the integration variables:

$$Q(z)=\int d\epsilon_1\int d\epsilon_2\int d\epsilon_1'\int d\epsilon_2' D(\epsilon_1)D(\epsilon_2)D(\epsilon_1')D(\epsilon_2')\times I(z|\epsilon_1,\epsilon_2|\epsilon_1',\epsilon_2')\{\epsilon_2+\epsilon_1'+\epsilon_2'\}\times\int d\epsilon\frac{D(\epsilon_1+\epsilon)-D(\epsilon_1-\epsilon)}{\epsilon}\quad . \tag{97}$$

The terms of Eq. (92) may now be evaluated numerically in the limit $\omega\to 0$ on the basis of Eqs. (79), (80), and (97) along with the definition (82) and the result (90). But first, we

check whether the Hall constant (92) reduces to the familiar expression $1/ne$, provided the electron density $n=(1/N)\Sigma_{\vec{k}\sigma}n_{\vec{k}\sigma}$ is very low. We concentrate on zero temperature, where we find the Fermi energy to be given by $n=1+\mathrm{erf}(\epsilon_F)$. This implies $\epsilon_F\to-\infty$ in the empty band limit. Then, the corrections on the rhs of Eq. (92) vanish and the Hall constant is given by Eq. (96). With $2a_{n0}=D(\epsilon_F)/\sqrt{d}$ and $2a_{d0}=-\epsilon_F D(\epsilon_F)/d$, we find in fact for $n\to 0$:

$$R_H=-\frac{\epsilon_F}{e\,D(\epsilon_F)}\simeq\frac{1}{en}\,. \tag{98}$$

E. Numerical results

First of all, we discuss the relative importance of the terms appearing on the rhs of Eq. (92). Figure 1 shows their doping dependence at $T=0$ (dashed lines) and that of their sum (solid line), where the doping parameter is defined as $\delta=1-n$. All functions vanish in the empty band limit ($\delta\to 1$) and exhibit monotonic behavior with decreasing doping. This reflects the fact, that the suppression of doubly occupied sites introduced by the Hubbard repulsion (3) becomes more effective with increasing electron density. As for the signs of the three contributions, only that of the two-point correlation function is negative. This, however, is sufficient to render the sum of all terms negative (solid line in Fig. 1). This remains valid at finite temperatures: The term K^{∞} is positive for all temperatures and doping levels considered, but is always overcompensated by the memory-function contribution $K^{II}(i0^+)+K^{III}(i0^+)$. Thus, our perturbation-theoretical results clearly indicate the tendency of the Hall constant to change its sign *below* half filling. However, for this to happen, the memory-function contribution must be taken into account.

To study the doping and temperature dependences of this precursor effect in greater detail, we shall extrapolate Eq. (92) to correlation strengths U big enough for the Hall constant to exhibit a sign change. Ultimately, we fix U such that this sign change occurs in the parameter regime observed experimentally in the case of the compound $La_{2-\delta}Sr_{\delta}CuO_4$. We shall measure U in terms of the bare bandwidth W, which may be chosen, due to Eq. (89), as $W=2t^*$ (from now on, the hopping parameter t^* is explicitly taken into account). Then, it follows from Eq. (92) and Fig. 1, that the $T=0$ threshold U, above which the Hall constant becomes positive, is $U=2.18W$ at half filling ($\delta=0$) and increases monotonically with increasing doping and ultimately diverges in the empty band limit $\delta\to 1$.

Before proceeding, we touch upon the issue of how to relate our theoretical results to experimental measurements. Firstly, the $d=\infty$ hopping parameter t^* has been estimated crudely as $0.2t^*\sim 500$ K.[20] Secondly, we shall express the Hall constant in units that allow the direct comparison with experimental results. This requires that charge carrier densities are taken with respect to the volume of a unit cell. On the other hand, the electron density n, appearing in Eq. (98), denotes the average number of electrons per lattice site. From a theoretical point of view, this definition is convenient since it is independent of the lattice dimension d and remains meaningful in the limit $d\to\infty$. Therefore, in order to compare our theoretical results with measurements on a certain cuprate, we have to multiply the Hall constant of Eq. (92) by Ω/ν, where Ω is the volume of a unit cell and ν the number of Cu ions therein. In the case of $La_{2-\delta}Sr_{\delta}CuO_4$, $\Omega=186$ Å^3 and $\nu=2$.

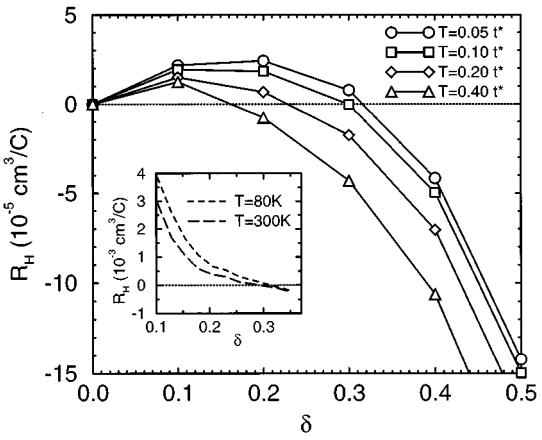

FIG. 2. Hall constant as a function of doping for $U=2.3\,W$. Inset: Data for polycrystalline samples of $La_{2-\delta}Sr_{\delta}CuO_4$ taken from Ref. 5.

After these preliminary remarks, we proceed with the investigation of the intermediate correlation regime, where a sign change is possible. Figure 2 shows the doping dependent Hall constant for several temperatures and the choice $U=2.3W$ (solid lines) as well as two experimental curves for polycrystalline samples of $La_{2-\delta}Sr_{\delta}CuO_4$ taken from Ref. 5 (inset). We see that the sign change occurs close to $\delta\approx 0.3$ for temperatures below 300 K, in agreement with experiment. For lower doping levels, our Hall constant exhibits a maximum and ultimately vanishes at half filling, irrespective of temperature. This reflects the fact that, in our perturbation-theoretical result (92), the Hall constant of the bare band is merely renormalized by a finite factor. Such a factor may change an overall sign but never can turn a vanishing quantity into a nonzero one. Thus perturbation theory fails to account for the observed $1/\delta$ law of the Hall constant near half filling. And that is why our perturbation-theoretical

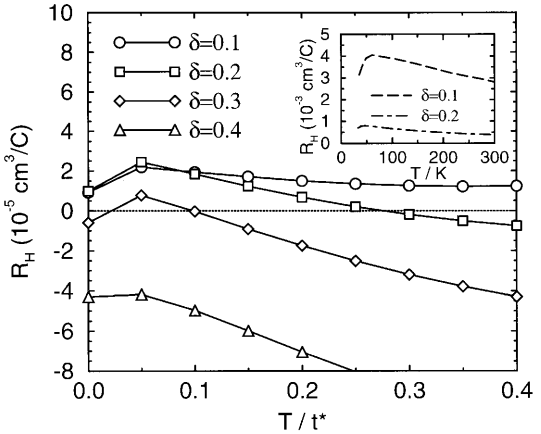

FIG. 3. Hall constant as a function of temperature for $U=2.3\,W$. Inset: Data for polycrystalline samples of $La_{2-\delta}Sr_{\delta}CuO_4$ taken from Ref. 11.

curves cross the zero line (dotted line in Fig. 2) with slopes that are two orders of magnitude smaller than those of the experimental curves. Apart from this deficiency of perturbation theory, the other dependences are in qualitative agreement with experiment. In Fig. 3, the temperature dependence of the Hall constant is shown for various doping levels within the range $0.1 \leqslant \delta \leqslant 0.4$ (solid lines) and compared to experimental results from Ref. 11, again for polycrystalline samples of $La_{2-\delta}Sr_{\delta}CuO_4$ (dashed lines in the inset). Despite the already mentioned difference in the order of magnitude of the Hall constant, our curves display the same features as the experimental ones: A maximum at low temperatures followed by a regime in which the Hall constant decreases monotonically up to unusually high temperatures. We have not been able to determine the exact location of the maximum due to numerical difficulties at nonzero temperatures below $0.05t^*$. Experimentally, it occurs above T_c. The fact that it appears within the Hubbard model suggests that it is not related to the onset of superconducting correlations. This is further supported by comparing the data of 90-K and 60-K $YBa_2Cu_3O_{6+x}$:[8] In this compound, the location of the maximum in $R_H(T)$ does not depend on the doping levels corresponding to the range $60\ \mathrm{K} < T_c < 90\ \mathrm{K}$. As for the decrease of the Hall constant as a function of temperature, it is experimentally found to be most pronounced at optimal doping, e.g., $\delta = 0.15$ in the case of $La_{2-\delta}Sr_{\delta}CuO_4$. Our results exaggerate the doping range where this decrease is markedly visible. At least, Fig. 3 shows that the decrease is least pronounced for the curve corresponding to the lowest doping level, $\delta = 0.1$. Furthermore, at high doping levels, where the memory-function contribution becomes unimportant, the Hall constant becomes almost temperature independent.

What about the observed quadratic dependence of the Hall angle on temperature for small doping levels?[8,10,11] This law cannot be verified on the basis of Eq. (92) alone, although, it cannot be falsified either. To make a check on this law, the longitudinal conductivity is needed as well. In principle, the calculation of this quantity can be done along the same lines leading to Eq. (92) and is left for future work.

IV. STRONG-CORRELATION REGIME

Numerical studies of multiband Hubbard models for the Cu-O planes of high-T_c materials indicate that all low-energy excitations are reproducible within a single-band Hubbard model with $U \sim W$.[21] Unfortunately, this parameter regime is not accessible to reliable analytical calculations. By contrast to the analysis of Sec. III, we shall now exaggerate the impact of U by considering the range $U \gg W$ instead. Henceforth, we shall assume a two-dimensional square lattice.

A. Hall constant in the crossover regime from $\omega \gg U$ to $\omega \ll U$

The main problem in dealing with the memory function of Eq. (33) is related to the fact that its dynamics is governed by the projected Liouville operator QLQ rather than L. We resolve this difficulty by inquiring into the properties of the memory function via its moments. Then, we may get rid of the superprojectors Q simply by resorting to their definition through Eq. (25) and thereafter.

1. The moments of the memory function in the limit $U \to \infty$

We start by rewriting the Hall constant (33) in terms of spectral functions:

$$R_H(z) = \frac{N}{e^2(\chi^0)^2 H} \int_{-\infty}^{\infty} d\omega \left\{ S_H(\omega) + K(\omega) \frac{\omega}{\omega - z} \right\}. \tag{99}$$

The first spectral function in the integrand is defined as

$$S_H(\omega) = -i\langle [\hat{J}_x, \delta(\omega + L)\hat{J}_y] \rangle , \tag{100}$$

and corresponds to the Hall matrix element of the current-current correlation function. The second function is related to the spectral function $M''(\omega)$, introduced in Eq. (43), by $K(\omega) = \chi^0 M''(\omega)/(\pi\omega)$, which implies

$$K(\omega) = \frac{-i\beta}{\omega} (QL\hat{J}_x | \delta(\omega + QLQ) | QL\hat{J}_y) \ . \tag{101}$$

This function describes the correlation between the residual forces $\hat{f}_x$ and $\hat{f}_y$. In the following, we shall uncover a simple connection between the moments of the two functions $S_H(\omega)$ and $K(\omega)$ in the limit $U \to \infty$.

First, we note that both functions may be shown to be even and real.[14] Furthermore, we expect both functions to vanish beyond a certain frequency above U, since U is the highest energy scale in the problem. This assumption will be corroborated below up to corrections of the order t/U. Hence, for finite but large U, all moments exist and it is sufficient, to consider only the even ones:

$$S_l = \int_{-\infty}^{\infty} d\omega \ S_H(\omega) \omega^{2l}, \tag{102}$$

$$K_l = \int_{-\infty}^{\infty} d\omega \ K(\omega) \omega^{2l}, \tag{103}$$

where $l \geqslant 0$. Since we are mainly interested in the dc-Hall constant, we would like to calculate K_0. Unfortunately, this is not feasible on the basis of Eq. (101), since the inverse of the projected Liouville operator QLQ does not exist. However, all the other moments (103) can be calculated: Due to Eq. (101), they are given as

$$K_l = i\beta (\hat{J}_x | \underbrace{LQL \ \ldots \ LQL}_{2l \text{ projectors } Q} | \hat{J}_y) \quad (l \geq 1) \ . \tag{104}$$

Now, if we insert $Q = 1 - P$, this expression decomposes into 4^l terms. Consider a special one consisting of p superprojectors P. By using the definition of P, this term is seen to decompose further into $f = p + 1$ factors of the form $\beta(\hat{J}|L^{m_j}|\hat{J})$, the orders of which are $U^{m_j - 1}$ due to the Kubo identity (19). Here, $\Sigma_{j=1}^{f} m_j = 2l + 1$. Thus, each factor lowers the relative order in U by one. Hence, the more superprojectors P a given term is composed of, the lower its relative order in U is. Therefore, all superprojectors Q may be removed from the rhs of Eq. (104) to leading order in t/U. And this, in turn, establishes the following relation between the $l \geqslant 1$ moments of Eqs. (102) and (103):

$$\frac{K_l}{U^{2l}} = -\frac{S_l}{U^{2l}} + o\left(\frac{t}{U}\right). \tag{105}$$

This equation does *not* imply that the functions (100) and (101) differ only by a sign in the limit $U \to \infty$. This conclusion would require positive or negative definite functions and finite moments even in the limit $U \to \infty$. None of both conditions is satisfied. To proceed anyway, we remind ourselves that in the context of the Hubbard model in the strong correlation limit, any spectral function is believed to separate into individual ''peaks'' centered around integer multiples of U (Refs. 22–24) (in this context, any connected structure of a given spectral function, irrespective of its detailed shape, is referred to as a ''peak;'' for instance, it may vanish at discrete points). This reflects the fact that one-particle excitations may be grouped into two Hubbard bands separated by the so-called charge-transfer gap, which is of the order U. Since the current operators produce particle-hole excitations, we expect the functions (100) and (101) to have peak structures centered around $\omega = 0$ and $\pm U$ related to excitations within the two Hubbard bands and across the charge-transfer gap, respectively. Therefore, these peaks are expected to have widths of the order of those of the Hubbard bands. In the following, we shall prove this picture at least for the function (100) and derive formulas required to extract more information from the relations (105).

2. Structure of the functions $S_H(\omega)$ and $K(\omega)$

The appropriate technique to investigate spectral properties of the Hubbard model in the strong-correlation limit was pioneered by Harris and Lange in the special case of single-particle excitations[22] and generalized by several other authors, see for instance Refs. 23 and 24. At the heart of this procedure stands the decomposition of a given operator into terms, which increase the number of doubly occupied sites by integer values p:

$$\hat{O} = \sum_{p=-\infty}^{\infty} \hat{O}_{pU}. \tag{106}$$

Together with the Lehmann representation of a given spectral function, one may then address the properties of its individual peaks. The decomposition (106) is accomplished by an iterative procedure based on a canonical transformation of the Hubbard Hamiltonian: $\hat{H} \to \exp\{i\hat{S}\}\hat{H}\exp\{-i\hat{S}\}$. The expansion of the operator $\hat{S}$ up to the order l in t/U eliminates those processes from $\hat{H}$ which change the total number of doubly occupied sites up to the order t^l/U^{l-1}. The corresponding transformed Hamiltonian $\hat{H}^{(l+1)}$ in turn helps to fix the next order of $\hat{S}$ in t/U and so on. Thus, subsequent iterations generate increasing orders in t/U. Once the generator $\hat{S}$ has been found to a given order, one may decompose any operator to the same order by first decomposing its rotated counterpart.[24]

In our case, t/U expansions may be terminated after the zeroth-order term since the relation (105) indicates that it is not sensible to go beyond. Then, we do not have to distinguish between original and transformed Fermi operators and the decomposition (106) specialized to the case of the operators $\hat{D}_{ij}^{\sigma} \equiv c_{i\sigma}^{+} c_{j\sigma}$, making up the components of the current operator, becomes

$$\hat{D}_{ij}^{\sigma} = \hat{D}_{ij;-U}^{\sigma} + \hat{D}_{ij;0}^{\sigma} + \hat{D}_{ij;U}^{\sigma}. \tag{107}$$

In terms of Hubbard operators $X_i^{0\sigma} \equiv c_{i\sigma}(1-\hat{n}_{i\bar{\sigma}})$, $X_i^{\sigma 0} \equiv (1-\hat{n}_{i\bar{\sigma}})c_{i\sigma}^{+}$, $X_i^{\bar{\sigma}2} \equiv c_{i\sigma}\hat{n}_{i\bar{\sigma}}$, and $X_i^{2\bar{\sigma}} \equiv \hat{n}_{i\bar{\sigma}}c_{i\sigma}^{+}$, where $\bar{\sigma} \equiv -\sigma$, the terms of Eq. (107) may be written conveniently as

$$\hat{D}_{ij;0}^{\sigma} = X_i^{\sigma 0} X_j^{0\sigma} + X_i^{2\bar{\sigma}} X_j^{\bar{\sigma}2}, \tag{108}$$

$$\hat{D}_{ij;-U}^{\sigma} = X_i^{\sigma 0} X_j^{\bar{\sigma}2}, \tag{109}$$

$$\hat{D}_{ij;U}^{\sigma} = X_i^{2\bar{\sigma}} X_j^{0\sigma}. \tag{110}$$

The Lehmann representation of the function (100) is derived straightforwardly:

$$S_H(\omega) = \frac{1}{Z}\sum_{n,m} M_{nm}(e^{-\beta\epsilon_n} - e^{-\beta\epsilon_m})\,\delta(\omega - [\epsilon_n - \epsilon_m]), \tag{111}$$

$$M_{nm} = \frac{1}{2i}\{\langle n|\hat{J}_x|m\rangle\langle m|\hat{J}_y|n\rangle - \langle n|\hat{J}_y|m\rangle\langle m|\hat{J}_x|n\rangle\}, \tag{112}$$

where states and energies are defined through the eigenvalue equation $(\hat{H} - \mu\hat{N})|n\rangle = \epsilon_n|n\rangle$. Inserting the decomposition of the current operators corresponding to Eq. (107), we find that the peak centered around $\omega = pU$ has a weight given by

$$W_{pU} = \frac{1}{2i}(\langle[\hat{J}_{x;pU}, \hat{J}_{y;-pU}]\rangle + \langle[\hat{J}_{x;-pU}, \hat{J}_{y;pU}]\rangle) \tag{113}$$

and that only the peaks $p = 0$ and $p = \pm 1$ survive in leading order in t/U.

We assume that the function (101) has qualitatively the same triple-peak structure. Although not proven, this assumption is shown to lead to reasonable conclusions.

3. Frequency dependence of the Hall constant in the range $\omega \gg W$

Given the peak structure of the functions (100) and (101), only the contributions of the satellite peaks around $\omega = \pm U$ can be resolved in the $l \geq 1$ moments (102) and (103) in lowest order in t/U. Thus, the relation (105) implies that the ''spectral weights'' of the peaks of $K(\omega)$ and $S_H(\omega)$ around $\omega = U$ differ only by a sign. Together with Eq. (99), we may then draw the following conclusions: For $\omega \gg U$, all peaks of $S_H(\omega)$ contribute to the Hall constant and none of $K(\omega)$. In the frequency range $W \ll \omega \ll U$, the high-frequency peaks cancel each other out while the contribution of the zero-frequency peak of $K(\omega)$ is negligible. Within this charge-transfer gap region, the frequency-dependent Hall constant is then lowered by a factor p in comparison to its infinite frequency limit,

$$R_H^{*} \equiv R_H(W \ll \omega \ll U) = p\, R_H^{\infty}, \tag{114}$$

if we define p to be the relative spectral weight of the low-energy structure of $S_H(\omega)$:

$$p=\frac{W_0}{W_{-U}+W_0+W_U}=\frac{\langle[\hat{J}_{x;0},\hat{J}_{y;0}]\rangle}{\langle[\hat{J}_x,\hat{J}_y]\rangle} \quad . \tag{115}$$

Equation (114) is valid except for corrections of the order t/U. Therefore, it is sufficient to evaluate it in the limit $U\rightarrow\infty$.

But first, we seek an interpretation of R_H^*. Inserting Eqs. (115) and (34) in Eq. (114) yields

$$R_H^*=\frac{N}{ie^2(\chi^0)^2}\lim_{H\rightarrow 0}\frac{\langle[\hat{J}_{x;0},\hat{J}_{y;0}]\rangle}{H} \quad , \tag{116}$$

which is to be evaluated in the limit $U\rightarrow\infty$. Therefore, expectation values are taken with respect to states without double occupancies. Then, the projected current operators take on the following form:

$$\hat{J}_{\nu;0}=it\sum_{\langle ij\rangle\sigma}\Delta_{ij}^{\nu}P_{ij}X_i^{\sigma 0}X_j^{0\sigma}, \tag{117}$$

since the term $X_i^{2\bar{\sigma}}X_j^{\bar{\sigma}2}$ of Eq. (108) may be omitted. Here, $\vec{\Delta}_{ij}\equiv\vec{R}_i-\vec{R}_j$ and P_{ij} is the phase factor defined in the text following Eq. (3). Since χ^0 is given by Eq. (95), we also need

$$\lim_{U\rightarrow\infty}a_n=\langle X_{\vec{R}}^{\sigma 0}X_{\vec{R}+\hat{x}}^{0\sigma}\rangle \ , \tag{118}$$

where $\hat{x}$ is a primitive lattice vector in the x direction. From Eqs. (116), (95), and (118), we conclude that R_H^* represents the infinite frequency Hall constant of the $U=\infty-$Hubbard model, which is defined as follows:

$$\hat{H}=-t\sum_{\langle ij\rangle\sigma}P_{ij}X_i^{\sigma 0}X_j^{0\sigma}. \tag{119}$$

In fact, the analysis of Sec. II is straightforwardly carried over to this model, the current operator of which is then found to be given by Eq. (117). Note that $p\neq 1$ expresses the fact that the limits $\omega\rightarrow\infty$ and $U\rightarrow\infty$ do not commute: If we start with the limit $\omega\rightarrow\infty$, the integral over $S_H(\omega)$ in Eq. (99) extends over all three peaks while when taking the limits in the reversed sequence, the high-energy peaks are unattainable from the outset.

Next, we derive an exact analytical expression for p by taking the additional limit $T\rightarrow\infty$. We may wonder whether this is reasonable. However, since the limit $U\rightarrow\infty$ was already carried out, at least, the condition $T\ll U$ is satisfied, i.e., the thermal energy cannot excite an electron across the charge-transfer gap. Furthermore, we expect neither of the high-frequency objects R_H^∞ and R_H^* to depend appreciably on temperature, since they correspond to and generalize the semiclassical expression for the Hall constant. In the context of high-temperature expansions, one has to cope with electrons or holes hopping around closed loops, which are defined by a sequence of adjacent lattice sites. Therefore, it is convenient not to expand the phase factors. Then, an electron hopping along a polygon $ijk\ldots li$ accumulates a phase proportional to the flux $\phi_{ijk\ldots li}$ enclosed. The procedure to expand expectation values of Hubbard operators like the nominator of Eq. (115) in powers of $1/T$ is explained, e.g., in Ref. 25. Using additionally Eq. (94) and

$$\lim_{U\rightarrow\infty}a_d=\langle X_{\vec{R}}^{\sigma 0}X_{\vec{R}+\hat{x}+\hat{y}}^{0\sigma}\rangle \ , \tag{120}$$

we obtain to leading order

$$p=\frac{1+\delta}{2} \ . \tag{121}$$

Although the high-temperature calculation has introduced another high-energy scale into our system, we expect this result to hold qualitatively for low temperatures as well. For instance it is expected that the difference between the plateau values of $R_H(\omega)$ on both sides of U increases monotonically as half filling is approached. Further down, we shall derive the same expression for p within a simple approximation valid at $T=0$.

Finally, we calculate R_H^∞ to leading order in $1/T$. The leading order of the amplitude Eqs. (118) and (120) is found to be $a_n=(\beta t/2)\delta(1-\delta)$ and $a_d=-(\beta^2t^2/4)\delta(1-\delta)(1-3\delta)$, respectively, which, when inserted into Eq. (93), results in

$$R_H^\infty=\frac{1}{|e|}\left(\frac{1-3\delta}{2}\right)\left(\frac{1}{\delta}+\frac{1}{1-\delta}\right) \ . \tag{122}$$

Together with Eqs. (114) and (121), we recover the result for R_H^* of Ref. 3 that was derived within the t-J model in leading order in $1/T$. In this work, it was further shown that, although R_H^* is renormalized as a function of T and J when including higher orders in $1/T$, the doping dependence of the Hall constant retains its most important features: its sign change at $\delta\approx 1/3$ and its singular behavior in the vicinity of half filling. What seems to be striking at first sight is the fact that the same properties are encountered for R_H^∞, i.e., the Hall constant at frequencies well beyond U. At such high frequencies, the *dynamics* of the electrons is insensitive to the interaction U. However, for nondynamical quantities as matrix elements, the correlations introduced by the Hubbard interaction remain important. Before we discuss possibilities to extend the moments technique to lower frequencies, we shall rederive the results of this subsection within a simple approximation, valid at $T=0$.

4. Hubbard I approximation

An expression for the frequency-dependent Hall conductivity with vertex corrections having been neglected was derived in Ref. 26:

$$\sigma_{xy}(z)=\frac{e^3H}{2}\sum_{k\sigma}\left[\frac{\partial\epsilon_{\vec{k}}}{\partial k_x}\right]^2\frac{\partial^2\epsilon_{\vec{k}}}{\partial k_y^2}\frac{\Pi_H(z,\vec{k})}{z} \quad , \tag{123}$$

$$\Pi_H(i\omega_m,\vec{k})\equiv\frac{1}{\beta}\sum_n G_{\vec{k}}(i\omega_n)^2[G_{\vec{k}}(i\omega_n+i\omega_m) - G_{\vec{k}}(i\omega_n-i\omega_m)]. \tag{124}$$

Here, the Green's function is given in terms of its spectral function as

$$G_{\vec{k}}(i\omega_n)=\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\,\frac{A_{\vec{k}}(\omega)}{i\omega_n-\omega}\,, \tag{125}$$

and e, in our notation, is negative. Furthermore, it is assumed that the momentum dependence arises solely from the dispersion $\epsilon_{\vec{k}}$ of the bare band. From Eq. (24), the definition (20) of the functions $\chi_{\nu\mu}(z)$, and the symmetry property $\chi_{yx}(z)=-\chi_{xy}(z)$,[15] we derive the following representation for the Hall conductivity:

$$\sigma_{xy}(z)=\frac{ie^2}{Nz}\,\beta\left\langle \hat{J}_x\left|\frac{L}{z+L}\right|\hat{J}_y\right\rangle\,. \tag{126}$$

Therefore, the function (100) may be connected to the Hall conductivity $\sigma_{xy}(\omega\pm i0^+)\equiv\sigma'_H(\omega)\pm i\sigma''_H(\omega)$ via

$$S_H(\omega)=N\frac{\omega\sigma''_H(\omega)}{\pi e^2}\,. \tag{127}$$

Since $\sigma''_H(\omega)$ arising from Eqs. (123) and (124) may be shown to be real and odd, the function (100) has indeed the correct analytic properties. Inserting Eqs. (124) and (125) into Eq. (123) and using Eq. (127), we obtain, after a standard calculation:[17]

$$S_H(\omega)=|e|H\sum_{\vec{k}}\left[\frac{\partial\epsilon_{\vec{k}}}{\partial k_x}\right]^2\frac{\partial^2\epsilon_{\vec{k}}}{\partial k_y^2}\,X_{\vec{k}}(\omega)\,, \tag{128}$$

$$X_{\vec{k}}(\omega)\equiv\int_{-\infty}^{\infty}\frac{d\omega_1}{2\pi}\int_{-\infty}^{\infty}\frac{d\omega_2}{2\pi}\,A_{\vec{k}}(\omega_1)A_{\vec{k}}(\omega_2)\times\left\{\frac{F_{\vec{k}}(\omega_1;\omega)-F_{\vec{k}}(\omega_2;\omega)}{\omega_1-\omega_2}+(\omega\to-\omega)\right\}\,, \tag{129}$$

$$F_{\vec{k}}(\epsilon;\omega)\equiv\frac{A_{\vec{k}}(\epsilon-\omega)}{2\pi}[f(\epsilon)-f(\epsilon-\omega)]\,. \tag{130}$$

By means of a partial integration, the corresponding sum rule is straightforwardly shown to be satisfied [cf. Eqs. (100), (94), and (86)].

Next, we evaluate Eqs. (128)–(130) in the so-called Hubbard I approximation:[27]

$$\frac{A_{\vec{k}}(\omega)}{2\pi}=\frac{1+\delta}{2}\;\delta\left(\omega-\frac{1+\delta}{2}\epsilon_{\vec{k}}\right)+\frac{1-\delta}{2}\;\delta\left(\omega-U-\frac{1-\delta}{2}\epsilon_{\vec{k}}\right)\,. \tag{131}$$

At $U=\infty$, only the first term contributes. Then, the quantity (129) becomes

$$X_{\vec{k}}(\omega)=2\left(\frac{1+\delta}{2}\right)^2\frac{\partial f\{[(1+\delta)/2]\epsilon_{\vec{k}}\}}{\partial\epsilon_{\vec{k}}}\,\delta(\omega)\,, \tag{132}$$

and by partial integration, we obtain

$$S_H(\omega;U=\infty)=\frac{1+\delta}{2}\,(-i\langle[\hat{J}_x,\hat{J}_y]\rangle)\,\delta(\omega)\,. \tag{133}$$

Here, the expectation value is given by Eqs. (94) and (86). The sum rule obeyed by $S_H(\omega)$ for $U\neq\infty$ implies $p=(1+\delta)/2$, as in Eq. (121). This provides further evidence that the result (121) may be trusted for all temperatures. Note, that in a real system, the function $S_H(\omega)$ must vanish at $\omega=0$. Only then do we obtain a finite Hall conductivity at $\omega=0$. The result (133) is an artifact of the vanishing width of the lower Hubbard band in Eq. (131). If we consider finite but large values of U, we may simulate the high-energy peaks of the function (100) by δ functions as well:

$$S_H(\omega;U\to\infty)=-i\langle[\hat{J}_x,\hat{J}_y]\rangle\left(\frac{1+\delta}{2}\,\delta(\omega)+\frac{1-\delta}{4}\times[\delta(\omega-U)+\delta(\omega+U)]\right)\,. \tag{134}$$

This may be proven by calculating the moments (102) in the limit $U\to\infty$.

Finally, we calculate R_H^∞ given by Eq. (93), analytically within the approximation (131) and at $U=\infty$. Although this has been done numerically some time ago,[28] our simple analytical treatment allows a direct comparison with the exact high-temperature result (122) and demonstrates that the resulting doping dependence does not rely on the location of the Fermi surface. This last point is blurred in the Boltzmann-equation-based approach of Ref. 4.

The amplitudes on the rhs of Eq. (93) are given by Eqs. (78) and (86). Thereby, the density is calculated to be

$$n_{\vec{k}\sigma}=\frac{1+\delta}{2}\;f\left(\frac{1+\delta}{2}\;\epsilon_{\vec{k}}\right), \tag{135}$$

since in Hubbard I approximation at $U=\infty$, only the first term on the rhs of Eq. (131) is to be kept. Momentum dependences arise solely from the dispersion $\epsilon_{\vec{k}}$ of the bare band, which is why we are looking for expressions for the functions $A(\epsilon)$ and $B(\epsilon)$, defined in Eqs. (87) and (88). These equations also exhibit the results in the limit of infinite dimensions, which we may take as smooth and convenient approximations. Except for the prefactors $1/\sqrt{d}$ and $1/d$, which ultimately cancel each other out, these expressions may be compared to those calculated numerically on a two-dimensional lattice. This reveals that here, the main effect of the limit $d\to\infty$ is to smooth out the logarithmic singularities at zero energy encountered in the case of the functions $D(\epsilon)$ and $B(\epsilon)$ in $d=2$. Therefore, this limiting procedure does certainly not affect the validity of our present analysis in any serious manner. At $T=0$, Eqs. (78), (86), (135), (87), and (88) imply

$$2a_n=\frac{1+\delta}{2\sqrt{d}}\,D\left(\frac{2\epsilon_F}{1+\delta}\right)\,, \tag{136}$$

$$2a_d=\frac{-\epsilon_F}{d}\,D\left(\frac{2\epsilon_F}{1+\delta}\right)\,. \tag{137}$$

A relation between the Fermi energy and the doping parameter is established straightforwardly, which, in terms of the function

$$H(\delta)\equiv\frac{2\epsilon_F(\delta)}{1+\delta}\ , \tag{138}$$

may be written as

$$\frac{1-3\delta}{1+\delta}=\mathrm{erf}(H(\delta))\ . \tag{139}$$

In summary, the function (93) at $U=\infty$ and $T=0$ may be written as follows:

$$|e|R_H^{\infty}=\frac{2}{1+\delta}\frac{H(\delta)}{D(H(\delta))}\ . \tag{140}$$

The most important features are first, at $\delta=1/3$, R_H^{∞} vanishes. Second, at $\delta\to 1$, we recover the exact result $R_H^{\infty}\simeq -1/(|e|(1-\delta))$. And third, at $\delta\to 0$, we find $R_H^{\infty}\simeq 1/(|e|2\delta)$. The last two statements are proven with the asymptotic relation $D^0(\epsilon)/\epsilon\simeq\pm 1-\mathrm{erf}(\epsilon)$, valid in the limit $\epsilon\to\pm\infty$. All these points are in exact agreement with Eq. (122). We take this as an indication that, on the one hand, the high-temperature result (122) remains qualitatively valid even at low temperatures, and, on the other, that the Hubbard I approximation is remarkably good in the case of the quantity (93). In Ref. 4, the doping dependence of the Hall constant in the Hubbard I approximation was discussed in terms of the Fermi surface. This is misleading for two reasons.

For one thing, the Hubbard I approximation misplaces the Fermi surface: The Luttinger theorem, which relates the volume enclosed by the Fermi surface to the electron density,[29] is violated in this approximation. In contrast to this, angle-resolved photoemission experiments on cuprates like $Nd_{2-x}Ce_xCuO_4$ (Refs. 30,31) appear to be consistent with local-density approximation band-structure calculations which, in turn, imply the validity of this theorem. Despite this flaw, the approximation (131) yields a doping dependence for the Hall constant which is in good agreement with experiments on $La_{2-x}Sr_xCuO_4$.

For another, it was pointed out in Refs. 3 and 32, that the high-frequency object R_H^{∞} is *not* directly related to the location and topology of the Fermi surface. Instead, in a strongly correlated system, the entire Brillouin zone tends to get populated. In consequence, the weighted density average (86) receives contributions from the entire Brillouin zone rather than just from the vicinity of the Fermi surface.

We can demonstrate this more explicitly by slightly changing the form of the lower Hubbard band in Eq. (131): We broaden the δ function a little bit and shift some relatively small amount Z of spectral weight to a new δ function contribution $Z\delta(\omega-L(\epsilon_{\vec{k}}))$, with the function $L(\epsilon_{\vec{k}})$ being undetermined yet. This amounts to replacing Eq. (135) by $n_{\vec{k}\sigma}=h(\epsilon_{\vec{k}})$ with the function $h(\epsilon_{\vec{k}})$ differing from $[(1+\delta)/2]f\{[(1+\delta)/2]\epsilon_{\vec{k}}\}$ only in the following respects: The step at $\epsilon_{\vec{k}}=2\epsilon_F/(1+\delta)$ and of height $(1+\delta)/2$ is smoothed out while a new, much smaller one of height Z occurs at $\epsilon_{\vec{k}}=L^{-1}(\epsilon_F)$. This last condition fixes the new Fermi surface. By choosing the function $L(\epsilon)$ appropriately, we may place the Fermi surface wherever we want. As long as $Z\ll(1+\delta)/2$, the crucial average $a_d=\int_{-\infty}^{\infty}d\epsilon\ B(\epsilon)h(\epsilon)$ does not differ very much from the result in Eq. (137). This reasoning illustrates that, in the presence of strong correlations, the doping dependence of R_H^{∞} is not necessarily correlated to the Fermi-surface location. Also note, that it does not matter whether the function $h(\epsilon)$ arises from coherent or incoherent excitations.

B. Hall constant in the low-frequency regime

In this section, we discuss the frequency dependence of the Hall constant for frequencies *below* the Mott-Hubbard gap. Therefore, the appropriate model to start with is the t-J model. It is straightforward to show that Eqs. (99)–(101) are still valid, however, with all quantities being redefined within the t-J model.[33] Apart from the redefinition of the Liouville operator, this amounts to replacing the canonical Fermi operators through projected ones in all quantities that appear, i.e., $c_{i\sigma}\to X_i^{0\sigma}$, and $c_{i\sigma}^{+}\to X_i^{\sigma 0}$. In particular, the current operator is then given by Eq. (117). If we renormalize the functions (100) and (101) according to

$$S_H(\omega;t-J)=-i\langle[\hat{J}_{x;0},\hat{J}_{y;0}]\rangle s(\omega)\ , \tag{141}$$

$$K(\omega;t-J)=-i\langle[\hat{J}_{x;0},\hat{J}_{y;0}]\rangle k(\omega)\ , \tag{142}$$

the analog of Eq. (99) reads

$$R_H(z)=R_H^{*}\left(1+\int_{-\infty}^{\infty}d\omega\ k(\omega)\ \frac{\omega}{\omega-z}\right)\ . \tag{143}$$

Here, R_H^{*} is the infinite frequency Hall constant of the t-J model that was already investigated in Ref. 3, and which has been introduced in Eq. (114) in the special case $J=0$. Furthermore, we have taken into account that the function $s(\omega)$ is normalized to unity, while $k(\omega)$ represents the unknown memory-function contribution. From the discussion in Sec. IV A 2, we expect the function $k(\omega)$ to have only one peak centered around zero frequency, because, in the t-J model, doubly occupied sites can occur only virtually. Before we set about discussing possibilities to calculate this function via its moments, we try to gain some phenomenological insight.

1. Phenomenological discussion

Very recently, the normal-state ac-Hall constant was measured in $YBa_2Cu_3O_7$ thin films for frequencies up to 200 cm^{-1}.[34] In this work, the experimental data have been fitted successfully in terms of parameters introduced by Anderson[12] to account for the observed T^2 dependence of the inverse Hall angle in high-T_c materials. Anderson's theory is based on spin-charge separation with two different relaxation times and effective masses associated with the spinon and holon degrees of freedom: τ_{tr} is the decay time of the holons with effective mass m_{tr}, scattering off thermally excited spinons. On the other hand, a transverse relaxation rate $1/\tau_H$ is determined by the scattering between the spinons. Apart from this, σ_{xx} and σ_{xy} have the ordinary Drude form, i.e., $\sigma_{xx}\propto\tau_{\mathrm{tr}}/m_{\mathrm{tr}}$ and $\sigma_{xy}=\sigma_{xx}\omega_c\tau_H$. Here, the cyclotron motion is characterized by a mass m_H, $\omega_c\propto 1/m_H$. In Ref. 34, Anderson's theory was extended to finite frequencies via the replacements $\tau_{\mathrm{tr}}\to\tau_{\mathrm{tr}}/(1-i\omega\tau_{\mathrm{tr}})$ and $\tau_H\to\tau_H/(1-i\omega\tau_H)$. This led to the following representation of the frequency-dependent Hall constant:

$$R_H(\omega)=\frac{m_{\rm tr}}{m_H}\frac{1}{ne}\left(1+\frac{\tau_H-\tau_{\rm tr}}{\tau_{\rm tr}}\frac{1}{1-i\omega\tau_H}\right) . \quad (144)$$

This result is equivalent to the exact expression (143), provided the following identifications are made:

$$k(\omega)=\frac{\tau_H-\tau_{\rm tr}}{\tau_{\rm tr}}L_{1/\tau_H}(\omega) , \quad (145)$$

$$R_H^*=\frac{m_{\rm tr}}{m_H}\frac{1}{ne} . \quad (146)$$

Here, $L_\Gamma(\omega)$ denotes the Lorentzian of width Γ normalized to unity. Therefore, the unusual relaxation time τ_H is a measure for the width of the function (142) and thus determines the decay rate of the correlation between the residual forces $\hat{f}_{x;0}$ and $\hat{f}_{y;0}$ of the t-J model [cf. Eqs. (31) and (101)]. Furthermore, the integrated weight of the function (145) measures the deviation of the relaxation time τ_H from the ordinary transport time $\tau_{\rm tr}$. This deviation is directly related to that of the Hall constant at zero frequency from its value at high frequencies:

$$\frac{\tau_H-\tau_{\rm tr}}{\tau_{\rm tr}}=\frac{R_H(\omega=0)-R_H^*}{R_H^*} . \quad (147)$$

In the phenomenological expression (144), the temperature dependence is entirely contained in the two relaxation rates. They are expected to vary as $\tau_{\rm tr}\propto 1/T$ and $\tau_H\propto 1/T^2$.[12] For dimensional reasons, we take $\tau_H\propto J/T^2$, since J is the only energy scale characteristic of our model. From these arguments, we may infer the following: For one thing, the memory-function does not only describe the unusual frequency dependence of the Hall constant in high-T_c superconductors. Also, the observed anomalous temperature dependence is mainly due to this memory-function contribution. For another, we expect $\tau_{\rm tr}$ to be relatively smaller than τ_H at low temperatures, since $\tau_H/\tau_{\rm tr}\propto J/T$. Thus, Eq. (147) suggests that the Hall constant *increases* when zero frequency is approached. This enhancement was actually observed in the above-mentioned measurements on $YBa_2Cu_3O_7$.[34] In any case, Eq. (147) indicates that the sign of the Hall constant is solely described by the high-frequency object R_H^*, as claimed in Ref. 3.

Does the discussion so far point towards spin-charge separation as advocated by Anderson? Obviously, the current operators $\hat{J}_\nu$ are related to the charge degrees of freedom only. Consequently, the spin physics must be accounted for by the residual forces $\hat{f}_\nu$. This is also reflected by the proportionality $\tau_H\propto J/T^2$. However, up to now, we do not have a compulsory argument why these residual forces should describe exclusively spin degrees of freedom.

In summary, Anderson's notion of two distinct relaxation rates is naturally backed up within the Mori theory. They may be interpreted as the time scales set by the current operators and their associated residual forces.

2. Moments approach to the memory function

Of course, it would be interesting to calculate the function $k(\omega)$ of Eq. (143) quantitatively within the t-J model in order to relate its width and its integrated weight to the parameters t, J, temperature T, and doping δ. From the above discussion, we expect that the relevant information about its overall form may be put into only few parameters. As already mentioned, even two parameters as in Eq. (145) have been sufficient to obtain an excellent fit of experimental data.[34] In this subsection, we suggest the following procedure to construct $k(\omega)$: Parametrize this function by n parameters which are subsequently fixed by its first n moments. Up to now, this seems to be the only reliable way to take into account the superprojectors Q. Of course, all moments

$$k_l=\int_{-\infty}^{\infty}d\omega\ k(\omega)\omega^{2l} \quad (148)$$

exist, which is why we have to replace the Lorentzian (145) by a ''short-range'' function, e.g., a Gaussian multiplied by a polynomial. We proceed by relating the moments of $k(\omega)$ to that of the function $s(\omega)$ and the optical conductivity. Finally, we discuss a possibility to calculate these moments.

The ordinary conductivity is given, according to Eq. (24), by the following expression:

$$\sigma_{xx}(\omega+i0^+)=\frac{ie^2}{N}\beta\left(\hat{J}_{x;0}\left|\frac{1}{\omega+L+i0^+}\right|\hat{J}_{x;0}\right) , \quad (149)$$

the real part of which may be shown to be an even function of ω,[14] and, due to a sum rule, can be written in terms of a function $c(\omega)$, that is normalized to unity:

$$\Re\{\sigma_{xx}(\omega+i0^+)\}=\pi e^2\chi^0 c(\omega)/N . \quad (150)$$

In Appendix D, we show that all the moments (148) may be traced back recursively to that of the functions (141) and (150):

$$s_l=\int_{-\infty}^{\infty}d\omega\ s(\omega)\omega^{2l} , \quad (151)$$

$$c_l=\int_{-\infty}^{\infty}d\omega\ c(\omega)\omega^{2l} , \quad (152)$$

provided $l\geqslant 1$. Thereby, only the definition of the superprojectors Q has to be used in Eq. (104). The result may be written as follows:

$$k_l=-s_l+\sum_{j=1}^{l}a_j s_{l-j} \quad \text{for} \quad l\geqslant 1 , \quad (153)$$

where the coefficients a_j are polynomials in the moments (152) and are listed in Appendix D up to $j=6$. If we had a good method for calculating the moments (151) and (152), we could construct the unknown function $k(\omega)$ via its first n moments as already explained. This approximation is reliable, if the zeroth moment k_0, calculated from Eq. (148), converges fast enough with increasing n. Since in the t-J model, $k(\omega)$ has only one peak around $\omega=0$, the first few moments are expected to be sufficient for this to happen. An advantage of this approach is that moments are *global* properties of a spectral function and as such are less sensitive to its detailed resonance structure and to approximations in-

volved. Also, some approximation schemes are better suited for the calculation of moments than the underlying spectral function.

For instance, within a high-temperature expansion, moments are accessible, at least in principle, while the corresponding spectral function is not. However, in the case of the moments (151), only very few moments, and to only low orders in $1/T$, are within reach. This is all the worse, since now, we are interested in the Hall constant at low frequencies, i.e., no other high-energy scale is present as it was in the context of R_H^*.

Another example is the exact diagonalization technique.[35] In this method, spectral functions are calculated numerically via the exact eigenstates and eigenenergies on the basis of their Lehmann representation. While being exact, the intrinsic problem of this method is the constraint of working on relatively small clusters. Therefore, the δ functions have to be broadened in order to obtain smooth functions. In contrast to this, no additional approximation is required when calculating moments. Of course, the smallness of the clusters remains the major restriction of this method. Nevertheless, when combined with the moments approach as suggested above, it is a means of extracting reliable information about the frequency-dependent Hall constant within the t-J model and should therefore be the subject of a future work.

V. DISCUSSION AND CONCLUSIONS

In summary, we have devised a memory-function approach to the Hall constant in strongly correlated electron systems, which enables us to cope directly with the Hall resistivity. We have focused our attention mainly on the memory-function term, which is neglected in Boltzmann-type approaches. The important physics to be expected from this contribution comprises the unusual frequency *and* temperature dependences of the Hall constant, observed in the normal state of high-T_c superconductors.

As a first step, the usefulness of our approach was demonstrated in a perturbation-theoretical treatment within the single-band Hubbard model. To obtain a regular expression for the memory-function contribution for all frequencies, we assumed that the subspace of the operator space spanned by the current operators $\hat{J}_x$ and $\hat{J}_y$ is invariant with respect to actions of the unperturbed Liouville operator. This approximation was shown to become exact in the continuum limit. Furthermore, it affects only the properties of the unperturbed system, i.e., the tight-binding electrons. Therefore, we do not expect the omitted terms to change the physics in an essential way. On the basis of this approximation, the memory function was calculated to leading order in the correlation strength U and shown to decompose into a two- and three-point correlation function, when expanded to first order in the magnetic field. The complicated expressions obtained for these two functions were simplified considerably by invoking the limit of infinite spatial dimensions. While this approximation still catches the impact of the correlations, it smoothes out effects of low dimensionality. Except for the doping dependence of the Hall constant in the vicinity of half filling, we have been able to reproduce the unusual experimental findings in connection with high-T_c superconductors as $La_{2-\delta}Sr_{\delta}CuO_4$. In particular, we could explain the sign change of the Hall constant as a function of doping and its decrease as a function of temperature up to unusually high temperatures. However, we had to choose $U=2.3W$ (W: bare bandwidth), which is, strictly speaking, outside the perturbative regime. Since the cuprates are believed to undergo a transition from a Fermi liquid to a strong-correlation regime when the doping approaches its optimal value from the overdoped side,[2] it is not astonishing that the $1/\delta$ law in the vicinity of the mother compound cannot be described within perturbation theory.

Therefore, we also considered the Hall effect in the opposite limit of strong correlations. In the single-band Hubbard model, a finite amount of spectral weight for particle-hole excitations, caused by the Hall current, is always pinned at the energy U. This is valid no matter how large the correlation strength U is. We have shown that the memory function removes these high-energy excitations in the limit $U\rightarrow\infty$, thus accounting for the frequency dependence of the Hall constant down to frequencies within the charge-transfer gap. The corresponding decrease of the Hall constant by a factor $(1+\delta)/2$ was calculated exactly to leading order in $1/T$ and corroborated within an approximate treatment, valid at $T=0$. However, our analysis did not provide us with information about the frequency dependence of the Hall constant at lower frequencies. The reason is that it was based on moments, which are dominated by the high-frequency contributions. We have also calculated the infinite frequency Hall constant analytically within the so-called Hubbard I approximation. In essence, we recovered the exact result for $U=\infty$ and $T\rightarrow\infty$ and explained, why this result does not rely on the location of the Fermi surface.

Finally, the Hall constant at low frequencies was investigated within the t-J model, an effective model acting in the reduced Hilbert space without doubly occupied sites. We observed that our memory-function formalism distinguishes inherently between two time scales: Firstly, the dynamics of the current operators is characterized by the ordinary transport relaxation time τ_{tr}. And secondly, the impact of all the other degrees of freedom on this charge transport is taken into account by fluctuating forces that introduce an unusual time scale τ_H. On the other hand, it was pointed out by Anderson, that temperature dependences of transport and Hall effect measurements can best be understood in terms of two relaxation times, following a $1/T$ and $1/T^2$ law.[12] We have shown that the time scales encountered within the Mori theory are identical to those introduced by Anderson. Furthermore, we have shown that the deviation of the unusual decay time τ_H from the ordinary transport time τ_{tr} is intimately connected to the frequency dependence of the Hall constant at low frequencies. Thus, the temperature and frequency dependence of the Hall constant result from each other and are both due to the memory-function contribution. It would be very interesting to investigate this interplay further, both theoretically and experimentally. As for the theoretical side, we have proposed an approach based on moments. It allows the exact treatment of the superprojector that reflects the distinction between the two time scales, leaving us with the problem of finding the first few moments of the ordinary current-current correlation functions. Except for a well studied prefactor, the memory-function term is mainly determined by two parameters. Therefore, we expect its first

few moments to provide us with enough information to fix these parameters.

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APPENDIX A: LATTICE SUMS OVER NEAREST NEIGHBORS

Since our gauge choice (9) permits periodic boundary conditions in the y direction only, we must carry out all sums over nearest neighbors according to the following formula:

$$\sum_{\vec{R},\vec{R}+\vec{\delta}} H(\vec{R},\vec{R}+\vec{\delta}) = \sum_{R_x}\sum_{R_y}\sum_{\delta_y} H(\vec{R},\vec{R}+\delta_y\,\hat{y}) + \sum_{\substack{R_x+\delta_x \\ R_x}}\sum_{R_y} H(\vec{R},\vec{R}+\delta_x\,\hat{x}) \quad . \tag{A1}$$

In the first term on the rhs, we may carry out the sum over R_y and δ_y independently. As for the second term on the rhs, we must make sure that R_x and $R_x+\delta_x$ are neighboring elements of the set $\{R_x^{\min}, R_x^{\min}+1, \ldots, R_x^{\max}\}$ with $R_x^{\max} \equiv R_x^{\min}+N_x-1$ as explained in the text following Eq. (12).

First of all, the matrices appearing in Eqs. (61), (63), and (72) are defined as follows:

$$B_\nu(\vec{k}_1,\vec{k}_2) = \frac{it}{N}\sum_{\vec{R},\vec{R}+\vec{\delta}} \delta_\nu\, e^{-i\vec{k}_1(\vec{R}+\vec{\delta})+i\vec{k}_2\vec{R}}, \tag{A2}$$

$$C(\vec{k}_1,\vec{k}_2) = \frac{1}{N}\sum_{\vec{R},\vec{R}+\vec{\delta}} (\delta_y)^2 R_x\, e^{-i\vec{k}_1(\vec{R}+\vec{\delta})+i\vec{k}_2\vec{R}}, \tag{A3}$$

$$D(\vec{k}_1,\vec{k}_2) = \frac{1}{N}\sum_{\vec{R},\vec{R}+\vec{\delta}} \delta_y R_x\, e^{-i\vec{k}_1(\vec{R}+\vec{\delta})+i\vec{k}_2\vec{R}} \quad . \tag{A4}$$

In all these cases, the integrand is proportional to a component of a nearest-neighbor vector, which entails that one of the two terms of Eq. (A1) vanishes. The summation over the y components R_y and δ_y is straightforward. In the case of Eqs. (A3) and (A4), the following sum is to be calculated:

$$\frac{1}{N_x}\sum_{R_x} R_x\, e^{i(k_{2x}-k_{1x})R_x} = \delta_{k_{1x}|k_{2x}} R_x^c + (1-\delta_{k_{1x}|k_{2x}}) \times \frac{e^{i(k_{2x}-k_{1x})R_x^{\min}}}{e^{i(k_{2x}-k_{1x})}-1} \quad , \tag{A5}$$

where $R_x^c \equiv (R_x^{\min}+R_x^{\max})/2$ is the x component of the lattice's center of gravity. In summary, we obtain the following results:

$$B_x(\vec{k}_1,\vec{k}_2) = \delta_{\vec{k}_1|\vec{k}_2} v_x(\vec{k}_1) + \delta_{k_{2y}|k_{1y}} \frac{it}{N_x} e^{i(k_{2x}-k_{1x})R_x^{\min}} \times (e^{ik_{1x}} - e^{-ik_{2x}}), \tag{A6}$$

$$B_y(\vec{k}_1,\vec{k}_2) = \delta_{\vec{k}_1|\vec{k}_2} v_y(\vec{k}_1), \tag{A7}$$

$$C(\vec{k}_1,\vec{k}_2) = 2\cos k_{1y}\,\delta_{k_{1y}|k_{2y}} \left(\delta_{k_{1x}|k_{2x}} R_x^c + (1-\delta_{k_{1x}|k_{2x}}) \times \frac{e^{i(k_{2x}-k_{1x})R_x^{\min}}}{e^{i(k_{2x}-k_{1x})}-1} \right), \tag{A8}$$

$$D(\vec{k}_1,\vec{k}_2) = -2i\sin k_{1y}\,\delta_{k_{1y}|k_{2y}} \left(\delta_{k_{1x}|k_{2x}} R_x^c + (1-\delta_{k_{1x}|k_{2x}}) \times \frac{e^{i(k_{2x}-k_{1x})R_x^{\min}}}{e^{i(k_{2x}-k_{1x})}-1} \right) . \tag{A9}$$

In the following section, we shall see that once these expressions are inserted into observable quantities, the final results become independent of the lattice location.

The commutators (49) and (51) are also calculated using Eq. (A1).

APPENDIX B: EVALUATION OF THE TWO- AND THREE-POINT CORRELATION FUNCTION

We begin by inserting Eqs. (61) and (63) into Eqs. (65) and (66) and by using Eqs. (74)–(76) along with Eqs. (A6)–(A9). Then, the correlation functions (65) and (66) are given as sums over terms that contain expectation values with respect to the momentum conserving Hamiltonian (14). Taking into account the corresponding δ functions, we see that the diagonal elements of the matrices (A6), (A8), and (A9) lead to vanishing contributions due to symmetry arguments. Moreover, the combination of all exponentials whose arguments are proportional to $R_x^{\min}$ may be replaced by one due to the δ functions, expressing momentum conservation in the model (14). With the help of the function

$$S(\vec{k}) = N_y \delta_{k_y|0}(1-\delta_{k_x|0}) \frac{1}{e^{ik_x}-1} = -\frac{1}{2} N_y \delta_{k_y|0} \left[1 + i\mathcal{P}\cot\left(\frac{k_x}{2}\right) \right] \tag{B1}$$

and after some straightforward manipulations, we arrive at

$$\frac{C^{II}(z)}{-2iHet^2NU^2}=\frac{1}{N^4}\sum_{\vec{k}_1\vec{k}_2\vec{q}\sigma}\sum_{\vec{k}'_1\vec{k}'_2\vec{k}'\vec{q}'\sigma'}\delta_{k_{2y}|k_{1y}-q_y}S(\vec{k}'_2+\vec{q}'-\vec{k}'_1)(e^{ik_{1x}}-e^{-i(k_{2x}+q_x)}-e^{i(k_{1x}-q_x)}+e^{-ik_{2x}})$$

$$\times[\cos k'_{1y}-\cos(k'_{1y}-q'_y)]\frac{\langle[\hat{A}^{\sigma}_{\vec{k}_1,\vec{k}_2|\vec{k}|\vec{q}},\hat{A}^{\sigma'}_{\vec{k}'_1,\vec{k}'_2|\vec{k}'|\vec{q}'}]\rangle_0^{(0)}}{z+\epsilon_{\vec{k}-\vec{q}}-\epsilon_{\vec{k}}+\epsilon_{\vec{k}_1}-\epsilon_{\vec{k}_2}} \quad , \tag{B2}$$

$$\frac{C^{III}(z)}{4iHet^3NU^2}=P_1(z)+P_2(z) \quad , \tag{B3}$$

$$P_1(z)=\frac{1}{N^4}\sum_{\vec{k}_1\vec{k}_2\vec{q}\sigma}\sum_{\vec{k}'_1\vec{k}'_2\vec{k}'\vec{q}'\sigma'}\sum_{p_1p_2\tau}S(\vec{p}_2-\vec{p}_1)\ \delta_{\vec{k}'_2+\vec{q}'-\vec{k}'_1|\vec{0}}\sin p_{1y}[\sin k'_{1y}-\sin(k'_{1y}-q'_y)](1-e^{-iq_x})$$

$$\times(e^{ik_{1x}}+e^{-ik_{2x}})\frac{e^{\beta(\epsilon_{\vec{p}_1}-\epsilon_{\vec{p}_2})}-1}{\epsilon_{\vec{p}_1}-\epsilon_{\vec{p}_2}}\frac{\langle c^{+}_{\vec{p}_1\tau}c_{\vec{p}_2\tau}\ [\hat{A}^{\sigma}_{\vec{k}_1,\vec{k}_2|\vec{k}|\vec{q}},\hat{A}^{\sigma'}_{\vec{k}'_1,\vec{k}'_2|\vec{k}'|\vec{q}'}]\rangle_0^{(0)}}{z+\epsilon_{\vec{k}-\vec{q}}-\epsilon_{\vec{k}}+\epsilon_{\vec{k}_1}-\epsilon_{\vec{k}_2}} \quad , \tag{B4}$$

$$P_2(z)=\frac{1}{N^4}\sum_{\vec{k}_1\vec{k}_2\vec{q}\sigma}\sum_{\vec{k}'_1\vec{k}'_2\vec{k}'\vec{q}'\sigma'}\sum_{p_1p_2\tau}S(\vec{p}_2-\vec{p}_1)\,\delta_{\vec{k}'_2+\vec{q}'-\vec{k}'_1|\vec{0}}$$

$$\times\frac{\sin p_{1y}[\sin k'_{1y}-\sin(k'_{1y}-q'_y)](1-e^{-iq_x})(e^{ik_{1x}}+e^{-ik_{2x}})}{(z+\epsilon_{\vec{k}-\vec{q}}-\epsilon_{\vec{k}}+\epsilon_{\vec{k}_1}-\epsilon_{\vec{k}_2})(z-\epsilon_{\vec{k}'-\vec{q}'}+\epsilon_{\vec{k}'}-\epsilon_{\vec{k}'_1}+\epsilon_{\vec{k}'_2})}\{\delta_{\tau|\sigma}[\,\delta_{\vec{p}_2|\vec{k}_1}\langle[\hat{A}^{\sigma}_{\vec{p}_1,\vec{k}_2|\vec{k}|\vec{q}},\hat{A}^{\sigma'}_{\vec{k}'_1,\vec{k}'_2|\vec{k}'|\vec{q}'}]\rangle_0^{(0)}$$

$$-\delta_{\vec{p}_1|\vec{k}_2}\langle[\hat{A}^{\sigma}_{\vec{k}_1,\vec{p}_2|\vec{k}|\vec{q}},\hat{A}^{\sigma'}_{\vec{k}'_1,\vec{k}'_2|\vec{k}'|\vec{q}'}]\rangle_0^{(0)}]+\delta_{\tau|-\sigma}[\,\delta_{\vec{p}_2|\vec{k}-\vec{q}}\langle[\hat{A}^{\sigma}_{\vec{k}_1,\vec{k}_2|\vec{k}|\vec{k}-\vec{p}_1},\hat{A}^{\sigma'}_{\vec{k}'_1,\vec{k}'_2|\vec{k}'|\vec{q}'}]\rangle_0^{(0)}$$

$$-\delta_{\vec{p}_1|\vec{k}}\langle[\hat{A}^{\sigma}_{\vec{k}_1,\vec{k}_2|\vec{p}_2|\vec{p}_2-\vec{k}+\vec{q}},\hat{A}^{\sigma'}_{\vec{k}'_1,\vec{k}'_2|\vec{k}'|\vec{q}'}]\rangle_0^{(0)}]\} \quad . \tag{B5}$$

From the definition (59), we find

$$[\hat{A}^{\sigma}_{\vec{k}_1,\vec{k}_2|\vec{k}|\vec{q}},\hat{A}^{\sigma'}_{\vec{k}'_1,\vec{k}'_2|\vec{k}'|\vec{q}'}]=\delta_{\sigma'|\sigma}c^{+}\vec{k}_1|\sigma c_{\vec{k}_2|\sigma}c^{+}_{\vec{k}'_1|\sigma}c_{\vec{k}'_2|\sigma}\{\delta_{\vec{k}|\vec{k}'-\vec{q}'}c^{+}_{\vec{k}-\vec{q}|-\sigma}c_{\vec{k}'|-\sigma}-\delta_{\vec{k}'|\vec{k}-\vec{q}}c^{+}_{\vec{k}'-\vec{q}'|-\sigma}c_{\vec{k}|-\sigma}\}$$

$$+\delta_{\sigma'|\sigma}\{\delta_{\vec{k}_2|\vec{k}'_1}c^{+}_{\vec{k}_1\sigma}c_{\vec{k}'_2\sigma}-\delta_{\vec{k}'_2|\vec{k}_1}c^{+}_{\vec{k}'_1\sigma}c_{\vec{k}_2\sigma}\}c^{+}_{\vec{k}'-\vec{q}'|-\sigma}c_{\vec{k}'|-\sigma}c^{+}_{\vec{k}-\vec{q}|-\sigma}c_{\vec{k}|-\sigma}$$

$$+\delta_{\sigma'|-\sigma}\{\delta_{\vec{k}|\vec{k}'_1}c^{+}_{\vec{k}-\vec{q}|-\sigma}c_{\vec{k}'_2|-\sigma}c^{+}_{\vec{k}'_1|\sigma}c_{\vec{k}_2|\sigma}c^{+}_{\vec{k}'-\vec{q}'|\sigma}c_{\vec{k}'|\sigma}$$

$$-\delta_{\vec{k}'|\vec{k}_1}c^{+}_{\vec{k}'-\vec{q}'|\sigma}c_{\vec{k}_2|\sigma}c^{+}_{\vec{k}'_1|-\sigma}c_{\vec{k}'_2|-\sigma}c^{+}_{\vec{k}-\vec{q}|-\sigma}c_{\vec{k}|-\sigma}\}$$

$$+\delta_{\sigma'|-\sigma}\{\delta_{\vec{k}_2|\vec{k}'-\vec{q}'}c^{+}_{\vec{k}_1\sigma}c_{\vec{k}'|\sigma}c^{+}_{\vec{k}'_1|-\sigma}c_{\vec{k}'_2|-\sigma}c^{+}_{\vec{k}-\vec{q}|-\sigma}c_{\vec{k}|-\sigma}-\delta_{\vec{k}'_2|\vec{k}-\vec{q}}c^{+}_{\vec{k}'_1|-\sigma}c_{\vec{k}|-\sigma}c^{+}_{\vec{k}_1|\sigma}c_{\vec{k}_2|\sigma}c^{+}_{\vec{k}'-\vec{q}'|\sigma}c_{\vec{k}'|\sigma}\} \quad . \tag{B6}$$

The further evaluation of Eqs. (B2), (B4), and (B5) requires the calculation of expectation values. Fortunately, not all terms that arise from the corresponding factorizations, contribute: Terms proportional to $\delta_{\vec{q}|\vec{0}}$ or $\delta_{\vec{q}'|\vec{0}}$ may be omitted in any case. And terms proportional to $\delta_{\vec{k}'_2|\vec{k}'_1-\vec{q}'}$ and $\delta_{\vec{p}_1|\vec{p}_2}$ do not contribute in the case of Eq. (B2) and Eq. (B4) along with Eq. (B5), respectively, due to the fact that $S(0)=0$. Thus, we see for example that a factor $f(\epsilon_{\vec{p}_1})[1-f(\epsilon_{\vec{p}_2})]$ may be split off from the expectation value within the integrand of Eq. (B4). This factor combines with the quotient that stems from the operator (73) according to

$$\frac{e^{\beta(\epsilon_{\vec{p}_1}-\epsilon_{\vec{p}_2})}-1}{\epsilon_{\vec{p}_1}-\epsilon_{\vec{p}_2}}f(\epsilon_{\vec{p}_1})(1-f(\epsilon_{\vec{p}_2}))=-\frac{f(\epsilon_{\vec{p}_1})-f(\epsilon_{\vec{p}_2})}{\epsilon_{\vec{p}_1}-\epsilon_{\vec{p}_2}} \quad . \tag{B7}$$

The further calculation is not simple and takes some time, especially in the case of the functions (B4) and (B5). In the thermodynamic limit, where we may replace, e.g., $N_y\delta_{k_y|0}\to 2\pi\delta(k_y)$, $(1/N)\Sigma_{\vec{k}}\to\int_{1.\,\mathrm{BZ}}d^dk/(2\pi)^d$, etc., our final result may be written in the form of Eqs. (77)–(84).

APPENDIX C: BRILLOUIN-ZONE AVERAGES IN INFINITE DIMENSIONS

The calculation of Brillouin-zone averages to leading order in $1/d$ follows the procedure outlined in Ref. 36. In the following, Schläfli's integral representation of the Bessel functions will play an important role:

$$\langle e^{ink+ir\cos k}\rangle_k = i^{|n|}J_{|n|}(r) \equiv G_n(r) \quad . \tag{C1}$$

Here, n is an integer and we have used the notation $\langle\cdots\rangle_k \equiv \int_{-\pi}^{\pi}\ldots\ dk/(2\pi)$. By means of the Fourier representation of the δ function, we may write, e.g., the function defined in Eq. (88) as follows:

$$B(\epsilon) = \int_{-\infty}^{\infty}\frac{ds}{2\pi}\ [iJ_1(r)]^2[J_0(r)]^{d-2}e^{is\epsilon} \quad , \tag{C2}$$

where here and in the following, $r \equiv s/\sqrt{d}$. Expanding the Bessel functions in powers of r and taking the limit $d\to\infty$, we find

$$B(\epsilon) = \frac{1}{4d}\frac{\partial^2}{\partial\epsilon^2}D(\epsilon) \quad . \tag{C3}$$

Thereby, we used $D(\epsilon) = \int_{-\infty}^{\infty}(ds/2\pi)e^{-s^2/4+is\epsilon}$, which is derived analogously. This proves Eq. (88). The corresponding evaluation of Eqs. (83) and (84) requires a Fourier series expansion of the cotangent:

$$\mathcal{P}\cot\left(\frac{k}{2}\right) = \frac{1}{i}\sum_{R\neq 0}\ \mathrm{sgn}(R)e^{ikR} \quad . \tag{C4}$$

Here, the sum is over all integers R, except for the zero. Since we are working in the thermodynamic limit, R may be considered to be a component of a lattice vector. To prove this representation, we start out with a known formula for the coefficients b_n appearing in the ansatz $\mathcal{P}\cot(k/2) = \Sigma_{n=1}^{\infty} b_n \sin(nk)$:

$$\frac{b_n}{2} = \mathcal{P}\int_{-\pi}^{\pi}\frac{dk}{2\pi}\ \cot\left(\frac{k}{2}\right)\sin(nk). \tag{C5}$$

With the substitution $z \equiv e^{ik}$, we may perform the principal value integration by invoking the theorem of residues: The integration contour goes around the unit circle with the point $z=1$ being excluded. Thus, we have to add the residue at $z=0$ to the half residue at $z=1$. We obtain $b_n = 2$ for all positive integers n, which proves the statement (C4). In the following, we show how the rhs of Eq. (84) is evaluated to leading order in $1/\sqrt{d}$. Writing the δ functions, that contain energies, in terms of Fourier integrals and introducing an additional momentum average $\langle (2\pi)^d \delta(\vec{k}+\vec{k}_2-\vec{k'}_1-\vec{k'}_2)\ \ldots\rangle_{\vec{k}} \equiv 1$, the problem reduces to the calculation of the following expression:

$$\left\langle e^{-i[s\epsilon_{\vec{k}}+s_1\epsilon_{\vec{k}_1}+s_2\epsilon_{\vec{k}_2}+s_1'\epsilon_{\vec{k}_1'}+s_2'\epsilon_{\vec{k}_2'}]} 2\pi\delta(k_x+k_{2x}-k'_{1x}-k'_{2x})\ 2\pi\delta(k_y-k_{1y})\prod_{j=3}^{d}2\pi\delta(k_j+k_{2j}-k'_{1j}-k'_{2j})\right.$$
$$\times\left\{\cos k_{1x}+\cos k_{2x}+\cos k'_{1x}+\cos k'_{2x}-[\sin k_{1x}+\sin k_{2x}-\sin k'_{1x}-\sin k'_{2x}]\ \mathcal{P}\cot\left(\frac{k_{1x}-k_x}{2}\right)\right\}$$
$$\left.\times\{\sin k_{1y}+\sin k_{2y}-\sin k'_{1y}-\sin k'_{2y}\}\sin k_{1y}2\pi\delta(k_{1y}+k_{2y}-k'_{1y}-k'_{2y})\right\rangle_{\vec{k}\vec{k}_1\vec{k}_2\vec{k}_1'\vec{k}_2'} . \tag{C6}$$

Since every dimension j contributes a term $-(1/\sqrt{d})\cos k_j$ to the band dispersion $\epsilon(\vec{k})$, the expression (C6) decomposes into d factors. For example, one factor arises from all x components:

$$\left\langle e^{i[r\cos k_x+r_1\cos k_{1x}+r_2\cos k_{2x}+r_1'\cos k'_{1x}+r_2'\cos k'_{2x}]}2\pi\delta(k_x+k_{2x}\right.$$
$$-k'_{1x}-k'_{2x})\Big\{\cos k_{1x}+\cos k_{2x}+\cos k'_{1x}+\cos k'_{2x}-[\sin k_{1x}$$
$$+\sin k_{2x}-\sin k'_{1x}-\sin k'_{2x}]$$
$$\left.\times\mathcal{P}\cot\left(\frac{k_{1x}-k_x}{2}\right)\Big\}\right\rangle_{k_x k_{1x}k_{2x}k'_{1x}k'_{2x}} . \tag{C7}$$

This expression decomposes further into eight terms corresponding to the ones in the curled brackets. Each has to be evaluated with the Fourier series expansion (C4) and that of the δ function:

$$2\pi\delta(k) = \sum_{R=-\infty}^{\infty} e^{ikR} \quad . \tag{C8}$$

For example, the term $-\sin k_{1x}\,\mathcal{P}\cot[(k_{1x}-k_x)/2]$ gives rise to the contribution

$$\sum_{n\neq 0}\sum_{m}\ \mathrm{sgn}(n)G_{m-n}(r)\frac{1}{2}[G_{n+1}(r_1)$$
$$-G_{n-1}(r_1)]G_m(r_2)G_m(r_1')G_m(r_2') \quad , \tag{C9}$$

where Eq. (C1) has been used. The leading order in $1/\sqrt{d}$ reads:

$$-G_1(r)G_0(r_1)G_0(r_2)G_0(r_1')G_0(r_2') \quad . \tag{C10}$$

This contribution to the expression (C6) is of order $1/\sqrt{d}$, as are all the others. The subsequent Fourier integrals over the variables s_i yield combinations of the functions (87), (88), and (89) thus leading ultimately to Eq. (91). Equation (90) is proven analogously.

APPENDIX D: REDUCTION OF THE MOMENTS OF THE MEMORY FUNCTION

First of all, we recall the definition of the moments (102) and (103), however with all operators and superoperators now being redefined within the t-J model. They are related to the moments (148) and (151) via the equations $K_l=-i\langle[\hat{J}_{x;0},\hat{J}_{y;0}]\rangle k_l$ and $S_l=-i\langle[\hat{J}_{x;0},\hat{J}_{y;0}]\rangle s_l$. In addition, we require the moments (152), renormalized as $C_l=\chi^0 c_l$. Next, we define the quantities

$$X_l^n := i\beta(L^n\hat{J}_{x;0}|\underbrace{LQ\ \ldots\ QL}_{l\text{ operators }L}|\hat{J}_{y;0}), \tag{D1}$$

$$Y_l^n := \beta(L^n\hat{J}_{x;0}|\underbrace{LQ\ \ldots\ QL}_{l\text{ operators }L}|\hat{J}_{x;0}), \tag{D2}$$

for $l\geq 1$. By using the definition for each of the first superprojector on the right-hand sides, we obtain the following recursion relations:

$$X_l^n=X_{l-1}^{n+1}-\frac{Y_1^n}{\chi^0}X_{l-1}^0 \quad \text{for } n \text{ odd}, \tag{D3}$$

$$X_l^n=X_{l-1}^{n+1}-\frac{X_1^n}{\chi^0}Y_{l-1}^0 \quad \text{for } n \text{ even}, \tag{D4}$$

$$Y_l^n=Y_{l-1}^{n+1}-\frac{Y_1^n}{\chi^0}Y_{l-1}^0 \quad \text{for } n \text{ odd}, \tag{D5}$$

$$Y_l^n=Y_{l-1}^{n+1} \quad \text{for } n \text{ even}. \tag{D6}$$

To prove these relations, we only have to use the following facts: X_1^n and Y_1^n vanishes for all odd and even integers n, respectively. This is due to the fact that the functions (100) and (150) are even, hence their odd moments vanish. Moreover, the quantities (D1) are of first order in the magnetic field. To relate the unknown moments K_l to the moments S_l and C_l, we have to supplement the recursion formulas (D3)–(D6) by the following equations:

$$K_l=X_{2l+1}^0, \tag{D7}$$

$$S_l=-X_1^{2l}, \tag{D8}$$

$$C_l=Y_1^{2l-1}. \tag{D9}$$

However, only even numbers of iterations occur. Therefore, we may combine two successive iteration steps into one. This leads to the following effective recursion relations:

$$H_l^n=H_{l-1}^{n+1}-\frac{C_{n+1}}{C_0}H_{l-1}^0+\frac{S_n}{C_0}N_{l-1}^1, \tag{D10}$$

$$N_l^n=N_{l-1}^{n+1}-\frac{C_n}{C_0}N_{l-1}^1, \tag{D11}$$

where we have defined

$$H_l^n := X_{2l+1}^{2n} \qquad \text{for } n\geq 0,\ l\geq 0, \tag{D12}$$

$$N_l^n := Y_{2l+1}^{2n-1} \qquad \text{for } n\geq 1,\ l\geq 0, \tag{D13}$$

and where the contact to the moments K_l, S_l, and C_l is established by means of the equations

$$K_l=H_l^0, \tag{D14}$$

$$S_l=-H_0^l, \tag{D15}$$

$$C_l=N_0^l. \tag{D16}$$

This recursive procedure results in Eq. (153) with the first six coefficients being given as follows:

$$a_1=2c_1, \tag{D17}$$

$$a_2=2c_2-3c_1^2, \tag{D18}$$

$$a_3=2c_3-6c_1c_2+4c_1^3, \tag{D19}$$

$$a_4=2c_4-6c_1c_3-3c_2^2+12c_1^2c_2-5c_1^4, \tag{D20}$$

$$a_5=2c_5-6c_1c_4-6c_2c_3+12c_1^2c_3+12c_1c_2^2-20c_1^3c_2+6c_1^5, \tag{D21}$$

$$a_6=2c_6-6c_1c_5-6c_2c_4+12c_1^2c_4-3c_3^2+24c_1c_2c_3 -20c_1^3c_3+4c_2^3-30c_1^2c_2^2+30c_1^4c_2-7c_1^6. \tag{D22}$$

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