THOULESS NUMBER AND SPIN DIFFUSION
IN QUANTUM HEISENBERG FERROMAGNETS

PETER KOPIETZ
Institut für Theoretische Physik der Universität Göttingen
Bunsenstr. 9, D-37073 Göttingen, Germany

ABSTRACT
Using an analogy between the conductivity tensor of electronic systems and the spin
stiffness tensor of spin systems, we introduce the concept of the Thouless number \( g_0 \) and
the dimensionless frequency dependent conductance \( g(\omega) \) for quantum spin models. It is
shown that spin diffusion implies the vanishing of the Drude peak of \( g(\omega) \), and that the
spin diffusion coefficient \( D_s \) is proportional to \( g_0 \). We develop a new method based on
the Thouless number to calculate \( D_s \), and present results for \( D_s \) in the nearest-neighbor
quantum Heisenberg ferromagnet at infinite temperatures for arbitrary dimension \( d \) and
spin \( S \).

1. Introduction
According to Thouless\(^1\) the conductivity of an electronic system of linear size \( L \) is a
measure of the rigidity of the wave functions with respect to a twist in the boundary
conditions. This is most clearly seen by writing the real part of the zero-frequency
limit of the dimensionless conductance in \( d \) dimensions,

\[
\tilde{g}(\omega) = \frac{L^{d-2} \sigma(\omega)}{e^2/\hbar},
\]

(1.1)
in the form\(^2\)

\[
\tilde{g}_0 \equiv \lim_{\omega \to 0} \text{Re} \tilde{g}(\omega) = \frac{\tilde{E}_c}{\Delta}.
\]

(1.2)

Here \( \Delta \) is the average spacing between energy levels at the Fermi energy, and \( \tilde{E}_c \)
is the Thouless energy, which is the typical fluctuation in energy levels caused by
replacing periodic with antiperiodic boundary conditions. In a system with a finite
diffusion coefficient \( D \), the Thouless energy is given by \( \tilde{E}_c = \hbar D/L^2 \), and can be
interpreted as \( \hbar \) divided by the time taken by a particle to diffuse across a box of
side \( L \). The dimensionless quantity \( \tilde{g}_0 \) is called Thouless number\(^3\). The metallic
state is defined by \( \tilde{g}_0 \gg 1 \), i.e. an electronic system is a metal if an interval of width
\( \tilde{E}_c \) around the Fermi energy contains many energy levels.
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In the present work we shall show that $\tilde{g}(\omega)$ has a precise dimensionless analog $g(\omega)$ in quantum spin systems, which can be very useful for a better understanding of spin diffusion. For simplicity we shall focus here on the spin-$S$ quantum Heisenberg ferromagnet, but it seems that our results can be generalized to Heisenberg antiferromagnets, and models of itinerant magnetism. The Hamiltonian of the nearest neighbor Heisenberg ferromagnet is given by

$$H = -J \sum_\mathbf{r} \sum_{\mu=1}^d \mathbf{S}_\mathbf{r} \cdot \mathbf{S}_{\mathbf{r} + \mathbf{a}_\mu},$$

(1.3)

where the $\mathbf{r}$-sum over the $N$ sites of a $d$-dimensional lattice, and $\mathbf{a}_\mu$, $\mu = 1, \ldots, d$, are vectors of length $a$ connecting site $\mathbf{r}$ with its nearest neighbor in direction $\mu$. We restrict ourselves to a hypercubic lattice, where $\mathbf{a}_\mu \cdot \mathbf{a}_\nu = a^2 \delta_{\mu\nu}$. $J > 0$ is the exchange coupling, and the $\mathbf{S}_\mathbf{r}$ are SU(2) spin operators satisfying $\mathbf{S}_\mathbf{r}^2 = S(S+1)$.

In their elegant quantum fluids approach to frustrated quantum antiferromagnets Chandra, Coleman, and Larkin\textsuperscript{4} recently introduced the notion of the dynamic spin stiffness tensor $K_{i\mu}^{\nu\mu}$, which is a tensor both in spin space and in real space. Here and below the indices $\mu, \nu = 1, \ldots, d$ refer to the $d$ directions in real space, and $i, j = x, y, z$ refer to the three components of the spin operators. A detailed discussion of the physical meaning of the spin stiffness tensor has been given in Ref.\textsuperscript{4} and will not be repeated here. Roughly, $K_{i\mu}^{\nu\mu}$ measures the energy change induced by a space- and time dependent local twist in the direction of the quantization axis of the spins. This definition is a generalization of the static spin stiffness $\rho^0_\mu$, which corresponds to a time-independent spiral twist of the quantization axis in the limit that the wavelength of the spiral becomes infinitely large\textsuperscript{5}. The existence of close analogies between the spin stiffness of classical Heisenberg models and the conductance of disordered electrons has first been noticed by Chakravarty\textsuperscript{6}. In Ref.\textsuperscript{7} we have derived a spectral representation for $K_{i\mu}^{\nu\mu}$ in quantum Heisenberg ferromagnets, and pointed out a formal similarity with the Kubo formula for the conductivity of electrons. Similar to the current response-kernel of an electronic system defined in the appendix, the spin stiffness tensor has a diamagnetic- and a paramagnetic part,

$$K_{i\mu}^{\nu\mu}(k, E) = D_{i\mu}^{\nu\mu} + P_{i\mu}^{\nu\mu}(k, E),$$

(1.4)

where $k^{-1}$ and $\hbar/E$ are the wavelength and time scale characterizing the local twist of the spin directions. To make the analogy with the electronic problem manifest, we define a mass $m_s$ by setting

$$\frac{\hbar^2}{m_s a^2} = J.$$

(1.5)

The diamagnetic part of the spin stiffness tensor can then be written as

$$D_{i\mu}^{\nu\mu} = -\delta_{i\mu} \delta_{j\nu} \frac{\hbar^2}{m_s L^2} \sum_\mathbf{r} < \mathbf{S}_\mathbf{r} \cdot \mathbf{S}_{\mathbf{r} + \mathbf{a}_\mu} - \mathbf{S}_\mathbf{r}^i \mathbf{S}_{\mathbf{r} + \mathbf{a}_\mu} >,$$

(1.6)
and the paramagnetic part $P_{\mu\nu}^{ij}(k, E)$ has the spectral representation

$$
P_{\mu\nu}^{ij}(k, E) = \sum_{n,m} p_n \left[ \frac{<n|J^i_{\mu}(k)|m> <m|J^j_{\nu}(-k)|n>}{E_m - E_n - E} + \frac{<n|J^j_{\nu}(k)|m> <m|J^i_{\mu}(-k)|n>}{E_m - E_n + E} \right].$$

(1.7)

Here $E_n$ and $|n>$ are exact eigenvalues and eigenstates of Eq. 1.3, $p_n$ are the Boltzmann factors $p_n = e^{-E_n/T}/Tr[e^{-H/T}]$, and $J_{\mu} = [J^x_{\mu}, J^y_{\mu}, J^z_{\mu}]$ is the spin current operator in direction $a_{\mu}$.

$$
J_{\mu}(k) = \frac{\hbar^2}{m_s L} \sum_r e^{ik \cdot r} \frac{1}{2a} \left[ S_r \times S_{r+a_{\mu}} - S_r \times S_{r-a_{\mu}} \right].
$$

(1.8)

The temperature $T$ is measured in units of energy. In $d$ dimensions one can define $3d$ spin currents, corresponding to the three spin projections and the $d$ directions in real space. In a temperature regime where the system has long-range spin correlations, the uniform spin stiffness $\rho_s^0$ is finite. In terms of the spin stiffness tensor defined above, $\rho_s^0$ is given by

$$
\rho_s^0 = -L^2 - \lim_{k \to 0} \left[ \lim_{\omega \to 0} K_{11}^{xx}(k, \hbar \omega + i0^+) \right].
$$

(1.9)

In case that the system has a spontaneous magnetization, we shall choose a coordinate system such that the direction defined by the magnetization is the $z$-direction in spin-space. From Eqs. 1.6 and 1.7 it is clear that the imaginary part of $K_{11}^{xx}(k, \hbar \omega + i0^+)$ vanishes at zero frequency, to that $\rho_s^0$ is real. At $T = 0$ Eq. 1.9 reduces to the familiar result $\rho_s^0 = a^2 - dJS^2$. For temperatures above the ordering temperature $T_c$, the diamagnetic- and paramagnetic contributions to $\rho_s^0$ precisely cancel, so that $\rho_s^0 = 0$. In fact, $\rho_s^0$ is the magnetic analog of the long-wavelength limit of the London-Kernel in an electronic system. Both quantities describe the appearance of a long-range rigidity in the wave functions. An obvious question, which apparently has not been discussed in the literature, is whether in a localized spin model one can also define the analog of the weight of the Drude peak in the expression for the conductivity of a metal. Furthermore, what is the analog of the Thouless number in spin systems? In the present paper we shall answer these questions.

2. Thouless number and spin conductance

Guided by the rescaled form of the Kubo formula for electrons given in the appendix, we define for the spin system the functions $g(\omega)$, $P(\omega)$, $K(\omega)$, and $K^*(k)$ by simply replacing in Eqs. A.3, A.6, A.8 and A.9 the rescaled current response kernel $K_{11}$ by the spin stiffness tensor $K_{11}^{xx}$,

$$
g(\omega) = \lim_{k \to 0} \frac{K_{11}^{xx}(k, \hbar \omega + i0^+)}{i(\hbar \omega + i0^+)}
$$

(2.1)
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\[ P(\omega) = \lim_{k \to 0} \frac{\text{Im} K_{11}(\omega, \hbar \omega + i0^+)}{\hbar \omega} \]  
\[ K(\omega) = -\lim_{k \to 0} \text{Re} K_{11}(\omega, \hbar \omega + i0^+) \]  
\[ K^s(k) = -\lim_{\omega \to 0} K_{11}(\omega, \hbar \omega + i0^+), \]  

We also define spin analogs \( K_0 \) and \( K_0^s \) of the weight of the Drude peak and the long-wavelength limit of the London kernel,

\[ K_0 = \lim_{\omega \to 0} K(\omega) \]  
\[ K_0^s = \lim_{k \to 0} K^s(k). \]

The function \( g(\omega) \) plays the role of the dimensionless conductance (see Eq.A.3), and we shall call \( g(\omega) \) "spin conductance". \( P(\omega) \) is the paramagnetic contribution to the real part of \( g(\omega) \) (see Eq.A.8), and the zero-frequency limit of \( K(\omega) \) yields the spin-analog of the weight of the Drude peak (see Eq.A.9). The wave-vector dependent function \( K^s(k) \) is related to the length-scale dependent spin stiffness \( \rho_s(k) = L^2 - d K^s(k) \), and corresponds to the London kernel of an electronic system (see Eq.A.6). A Schwinger-Boson calculation of \( \rho_s(k) \) for the two-dimensional quantum ferromagnet has been given in Ref.7. Because the imaginary part of \( K_{11}(\omega, \hbar \omega + i0^+) \) vanishes, it is not necessary to take the real part on the right-hand side of Eq.2.4

We now connect the above definitions with the phenomenon of spin diffusion. It is easy to obtain the following exact spectral representations,

\[ P(\omega) = \pi \left( 1 - e^{-\hbar \omega/T} \right) \frac{\text{Im} \sum_{n,m} p_n \delta(E_m - E_n - \hbar \omega)}{\hbar \omega} \]  
\[ K(\omega) = \frac{\hbar^2}{m_s L^2} \sum_r <S^z_r S^z_{r+a_1} + S^y_r S^y_{r+a_1}> \]  
\[ -\lim_{k \to 0} \frac{\text{P} \left\{ \frac{p_n - p_m}{E_m - E_n - \hbar \omega} \right\}}{\sum_{n,m} <n|J_{1}^s(k)|m>^2}, \]  

where \( \text{P} \) denotes the Cauchy principal value. General hydrodynamic arguments tell us that spin diffusion can only exist in the paramagnetic regime \( T \geq T_c \). In this case the low-frequency and long-wavelength behavior of the dynamic structure factor \( S(k, \omega) \) is of the form

\[ S(k, \omega) = 2\pi \hbar \sum_{n,m} p_n \delta(E_m - E_n - \hbar \omega) |<n|S^z_k|m>|^2 \]  
\[ = 2\chi \left[ \frac{\hbar \omega}{1 - e^{-\hbar \omega/T}} \right] \frac{\hbar D_s k^2}{(\hbar D_s k^2)^2 + (\hbar \omega)^2} , \]  

where \( D_s \) is the spin diffusion coefficient, and \( \chi = T^{-1} \sum_r <S^z_0 S^z_r> \) is the uniform susceptibility. The Fourier transform of the spin operators is defined by
\( S_k = N^{-1/2} \sum_r e^{ik \cdot r} S_r \). The Heisenberg equation of motion for \( S_k \) yields
\[
\hbar \frac{\partial S_k}{\partial t} = \frac{J}{\sqrt{N}} \sum_q S_q \times S_{k-q} \sum_{\mu=1}^d \cos [(k-q) \cdot a_\mu] ,
\]
where the momentum sum is over the first Brillouin zone. On the other hand, Fourier transformation of the right-hand side of Eq.1.8 yields
\[
J_\mu(k) = \frac{iJ}{L} \sum_q S_q \times S_{k-q} \sin [(k-q) \cdot a_\mu],
\]
where we have used \( \hbar^2 / (m_s a^2) = J \). Combining Eqs.2.10 and 2.11 and taking matrix elements we obtain to leading order in \( |k \cdot a_\mu| \ll 1 \)
\[
(E_n - E_m) < n|S_k| m > = L \sum_{\mu=1}^d < n|J_\mu(k)| m > k \cdot a_\mu .
\]
Inserting this into Eq.2.7 we arrive at
\[
P(\omega) = N \frac{(\hbar \omega)^2}{2\hbar} \left[ 1 - e^{-\hbar \omega / T} / \hbar \omega \right] \lim_{k \to 0} S(k, \omega) / (kL)^2 .
\]
Finally, using the assumption of the diffusive form of \( S(k, \omega) \) given in Eq.2.9, we obtain
\[
\lim_{\omega \to 0} P(\omega) = \frac{N}{L^2} \chi D_s, \quad (2.14)
\]
To complete the analogy with the electronic system, we should also prove that spin diffusion implies the vanishing of the weight of the Drude peak \( K_0 \) defined in Eq.2.3.
To show this, we use the following trick: We know that for \( T > T_c \) the uniform spin stiffness \( \rho_0^s \) vanishes \({\ref{2.6})}, so that
\[ K_0^s = - \lim_{k \to 0} \lim_{\omega \to 0} K_{11}^s(k, \omega) = 0. \]
Hence \( K_0 = K_0^s - K_0^s \) for \( T > T_c \). But the diamagnetic part \( D_{ij}^\mu \) of the spin stiffness tensor is independent of momenta and frequency, and does not appear in the difference \( K_0 - K_0^s \), so that
\[
K_0 - K_0^s = \lim_{k \to 0} \lim_{\omega \to 0} \lim_{\omega \to 0} \sum_{n,m} \frac{P_n - P_m}{E_m - E_n - \hbar \omega} \left| n|J_\mu(k)| m > \right|^2 .
\]
The contribution from all non-degenerate states \( E_n \neq E_m \) cancels on the right-hand side of this identity, because in this case the zero-frequency limit is harmless and we may interchange the order of the limits. Degenerate states contribute only if the limit \( \omega \to 0 \) is taken before the limit \( k \to 0 \), because for finite \( \omega \) we have \( \lim_{E_m \to E_n} (P_n - P_m)/(E_m - E_n - \hbar \omega) = 0 \). Hence
\[
K_0 - K_0^s = \frac{1}{T} \sum_{n,m} \frac{P_n}{E_n = E_m} \left| n|J_\mu(k)| m > \right|^2 .
\]

Using the identity
\[
\sum_{n,m} = \lim_{\omega \to 0} \hbar \int_{-\omega}^{\omega} d\omega' \sum_{n,m} \delta(E_m - E_n - \hbar \omega'),
\]
and comparing the right-hand side of Eq. 2.16 with the spectral representation of
\[P(\omega)\] in Eq. 2.7, we conclude that
\[
K_0 = \frac{\hbar}{\pi} \lim_{\omega \to 0} \int_{-\omega}^{\omega} d\omega' P(\omega') + K_s^0.
\]
Using now the fact that according to Eq. 2.14 \[P(\omega)\] has a finite limit as \(\omega \to 0\),
and that \(K_s^0 = 0\) for \(T > T_c\), we see that the right-hand side of Eq. 2.18 vanishes,
so that \(K_0 = 0\). The vanishing of the Drude peak in the presence of diffusion is
familiar from the electronic problem, see Eq. A.12. The Thouless number of a spin
system with spin diffusion is then
\[
g_0 = \lim_{\omega \to 0} \text{Re} g(\omega) = \frac{E_c}{\Delta},
\]
where \(\Delta = (N\chi)^{-1}\) plays the role of the level spacing \(\hat{\Delta}\) of the system,
and the Thouless energy for the spin system is again defined by \(E_c = \hbar D_s/L^2\).

3. Spin Diffusion

3.1. General remarks

First of all, it should be emphasized that there exists no proof of spin diffusion in
Heisenberg ferromagnets. Our calculations in Sec. are based on the assumption
that the long-wavelength and low-frequency behavior of the dynamic structure factor is
of the diffusive form given in Eq. 2.9. The fact that even for temperatures large
compared with \(J\) the spin diffusion problem is highly non-trivial is most clearly
seen by writing the spin diffusion coefficient in the form (see Eqs. 2.7 and 2.14)
\[
\hbar D_s a^{-2} = \pi J \lim_{\Omega \to 0} \lim_{N \to \infty} \int_{-\infty}^{\infty} d\epsilon \frac{\text{Tr}_N \left\{ e^{-\beta H} \hat{1} \delta(\Omega + \epsilon - \hat{H}) \hat{1} \delta(\epsilon - \hat{H}) \right\}}{\text{Tr}_N \left\{ e^{-\beta \hat{H}} \right\}},
\]
where \(\beta = J/T\), and \(\text{Tr}_N\) denotes the trace over the Hilbert space of the \(N\)-site
Heisenberg model, and the dimensionless operators \(\hat{H} = \hat{H}_x + \hat{H}_y + \hat{H}_z\) and \(\hat{1}\) are
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given by

\[ \hat{H}^i = - \sum_r \sum_{\mu=1}^d S^i_r S^{i\mu}_{r+a_\mu}, \quad i = x, y, z \]  \hspace{1cm} (3.2)

\[ \hat{I} = \frac{1}{\sqrt{N}} \sum_r S^y_r \left[ S^z_{r+a_1} - S^z_{r-a_1} \right] \]  \hspace{1cm} (3.3)

From Eq.3.1 it is obvious that a finite spin diffusion coefficient can only be obtained in an infinite system. In any finite system the trace in Eq.3.1 will consist of a sum of \( \delta \) functions, so that \( D_s \) cannot be defined. See Ref.\( ^1 \) for a discussion of this point for the electronic problem. Moreover, even after taking the thermodynamic limit \( N \to \infty \), it is not clear that the right-hand side of Eq.3.1 reduces to a finite constant. In principle, there are three possibilities, familiar from disordered electronic systems:

1) **Perfect conductor.** Eq.3.1 contains two \( \delta \)-functions, but only one energy integration. If the current operators would commute with the Hamiltonian, then the right-hand side of Eq.3.1 would be proportional to \( \delta(\Omega) \), so that the spin conductance has a Drude-peak, and spin diffusion does not occur. In this case the system behaves like a perfect conductor. Although in the Heisenberg model \( [\hat{I}, \hat{H}] \neq 0 \), there exists no proof that the non-commutativity is sufficient to remove the Drude peak.

2) **Metal.** In this regime the Thouless number \( g_0 \) and the spin diffusion coefficient are finite, and are related via Eq.2.13.

3) **Insulator.** The third possibility is that in a certain parameter regime the right-hand side of Eq.3.1 scales to zero in the thermodynamic limit. This would correspond to the insulating state of a disordered electronic system.

**3.2. Spin diffusion at infinite temperature**

We now assume that the spin diffusion coefficient is finite and develop a transparent and direct method to calculate \( D_s \) at infinite temperatures. The problem of calculating \( D_s \) at \( T = \infty \) has been studied intensely more than 20 years ago. Most methods are based on an indirect calculation of \( D_s \) via the dynamic structure factor \( S(k, \omega) \), assuming that its long-wavelength and low-frequency behavior is of the form given in Eq.2.9. The spin diffusion coefficient is obtained indirectly from \( S(k, \omega) \) by means of the limiting procedure \( \lim_{\omega \to 0} \lim_{k \to 0} (\omega^2/k^2) S(k, \omega) \), see Eq.2.9.

In praxis, it is impossible to calculate \( S(k, \omega) \) at low-frequencies, or equivalently its real-time Fourier transform \( S(k, t) \) at long times \( t \). The moment method first applied by de Gennes is equivalent to an extrapolation of a short time expansion to long times. The concept of the Thouless number in spin systems offers a more direct way to calculate \( D_s \). Of course, if \( S(k, \omega) \) could be calculated exactly, then the result for \( D_s \) would be identical with the result obtained by means an exact calculation of \( g(\omega) \). However, extrapolations of high-frequency expansions of \( g(\omega) \) and \( S(k, \omega) \) will in general not agree, because only in the limit \( \omega \to 0 \) and \( k \to 0 \)
there is a direct connection between these two quantities. We believe that our approach via the Thouless number $g_0$ is more reliable than extrapolations based on the dynamic structure factor, because $g_0$ is directly proportional to $D_s$, and no further limiting procedures are required.

We now use the first two expansion coefficients in the short time expansion of the right-hand side of Eq. 3.1 to estimate $D_s$ at $T = \infty$. Introducing Fourier representations of the $\delta$-functions and defining $\hat{I}(t) = e^{i\hat{H}t}\hat{I}e^{-i\hat{H}t}$, we obtain from Eq. 3.1 after straightforward manipulations

$$\hat{h}D_s a^{-2} = \frac{J}{T\chi} \int_0^{\infty} C(t)$$

(3.4)

$$C(t) = \frac{1}{2} \langle \hat{I}(0) [\hat{I}(t) + \hat{I}(-t)] \rangle,$$

(3.5)

where $\langle \cdots \rangle$ denotes thermal average with the Hamiltonian $\hat{H}$. The existence of the integral in Eq. 3.5 implies spin diffusion. The convergence of the integral is determined by the long-time behavior of $C(t)$. Unfortunately, there exists no completely controlled method to calculate $C(t)$ for large $t$. We therefore assume that the integral exists, and try to extract the long-time behavior from the short-time expansion,

$$C(t) = \sum_{n=0}^{\infty} \frac{(-1)^n t^{2n}}{(2n)!} C_{2n}.$$

(3.6)

Note that only even powers of $t$ appear, because $C(t) = C(-t)$. The expansion coefficients $C_{2n}$ can be written in terms of multiple commutators. The first two coefficients are

$$C_0 = \langle \hat{I}^2 \rangle,$$

(3.7)

$$C_2 = \langle \hat{I} \left[ \hat{I}, \hat{H} \right], \hat{H} \rangle,$$

(3.8)

where all operators are at equal times. At $T = \infty$ the evaluation of the thermal averages in Eqs. 3.7 and 3.8 simplify, because spins at different sites are not correlated. To calculate $C_0$, we need $\langle (S^i)^2 \rangle = S(S+1)/3$, for $i = x, y, z$. A short calculation gives

$$C_0 = 2 \left[ \frac{S(S+1)}{3} \right]^2.$$

(3.9)

The evaluation of $C_2$ is tedious but not difficult. It involves the expectation values of up to four spins, which have been tabulated in Ref. 14. The following averages are needed

$$\langle S^i S^j S^k \rangle = \frac{\delta^{ij} \delta^{jk} - \delta^{ik} \delta^{ij}}{6} S(S+1),$$

(3.10)

$$\langle (S^i)^4 \rangle = \frac{S(S+1)}{15} [3S(S+1) - 1],$$

(3.11)
where \( < \ldots > = \text{Tr}[\ldots]/(2S + 1) \), and the trace is over the \( 2S + 1 \) states of the spin-\( S \) Hilbert space. \( \epsilon^{ijk} \) is the antisymmetric Levi-Civita tensor. For \( i \neq j \) we have

\[
< (S^i)^2(S^j)^2 > = \frac{S(S + 1)}{15} \left[ S(S + 1) + \frac{1}{2} \right],
\]

\( \text{(3.12)} \)

\[
< S^iS^jS^iS^j > = \frac{S(S + 1)}{15} [S(S + 1) - 2].
\]

\( \text{(3.13)} \)

Writing

\[
C_2 = \sum_{i,j=x,y,z} C_{ij}^2 = \sum_{i,j=x,y,z} < \hat{I}_i [\hat{H}^i, \hat{H}^j] > .
\]

\( \text{(3.14)} \)

we obtain for a \( d \)-dimensional hypercubic lattice

\[
C_{xx}^2 = \left[ \frac{S(S + 1)}{3} \right]^2 \left[ (2d - \frac{2}{5}) \frac{4S(S + 1)}{3} - \frac{3}{5} \right],
\]

\( \text{(3.15)} \)

\[
C_{yy}^2 = C_{zz}^2 = \left[ \frac{S(S + 1)}{3} \right]^2 \left[ (d - \frac{3}{5}) \frac{4S(S + 1)}{3} - \frac{2}{5} \right],
\]

\( \text{(3.16)} \)

and \( C_{xy}^2 = C_{yx}^2 = C_{xz}^2 = C_{zx}^2 = 0 \). Hence

\[
C_2 = \left[ \frac{S(S + 1)}{3} \right]^2 \left[ (4d - 2) \frac{4S(S + 1)}{3} - 1 \right].
\]

\( \text{(3.17)} \)

We are now ready to extrapolate \( C(t) \) to long times. This extrapolation is of course not unique. A widely used extrapolation scheme, which we shall follow here, is to assume that the first two coefficients are consistent with a Gaussian. This leads to

\[
C(t) \approx C_0 \exp \left[ -\frac{C_2 t^2}{2C_0} \right].
\]

\( \text{(3.19)} \)

Using the fact that \( T\chi = S(S + 1)/3 \) at \( T = \infty \), we finally obtain from Eqs. 3.4, 3.9, 3.18 and 3.19 for the spin diffusion coefficient at \( T = \infty \)

\[
\frac{\hbar D_s}{a^2 J} = \left[ \frac{\pi S(S + 1)}{3} \right]^{1/2} \left[ 4d - 2 - \frac{3}{4S(S + 1)} \right]^{-1/2}.
\]

\( \text{(3.20)} \)

This is the main result of this section. Note that the term proportional to \( [S(S + 1)]^{-1} \) in the second factor of Eq. 3.20 can be viewed as a quantum correction, that becomes irrelevant in the limit of large \( S \). For \( S = 1/2 \) Eq. 3.20 reduces to

\[
\frac{\hbar D_s}{a^2 J} = \frac{1}{2} \left[ \frac{\pi}{4d - 3} \right]^{1/2} = \begin{cases} 0.886 & \text{for } d = 1 \\ 0.396 & \text{for } d = 2 \\ 0.295 & \text{for } d = 3 \end{cases}
\]

\( \text{(3.21)} \)
The classical limit of the Heisenberg model should be taken by letting $S \to \infty$ while keeping $J_{cl} = JS^2$ constant. In this limit $D_s$ vanishes. The leading coefficient for large $S$ can be read off from Eq. 3.20.

$$\frac{\hbar D_s}{a^2 J_{cl}} = \frac{1}{S} \left[ \frac{\pi}{4d - 2} \right]^{1/2} = \frac{1}{S} \times \begin{cases} 0.724 & \text{for } d = 1 \\ 0.418 & \text{for } d = 2 \\ 0.324 & \text{for } d = 3 \end{cases} \quad (3.22)$$

Eq. 3.21 agrees with the results listed in the first column of table V of Ref. 13. Hence, at least to second order in the short time expansion, our method is equivalent with Morita’s memory function formalism 13. However, it seems that our Thouless-number approach is physically more transparent, because it does not involve the construction of momentum dependent auxiliary quantities. The results in $d = 3$ are also in excellent agreement with Bennett and Martin 11, who obtained by means of an indirect extrapolation method based on the dynamic structure factor $\hbar D_s/(a^2 J) \approx 0.33 \sqrt{S(S + 1)}$. This gives $\hbar D_s/(a^2 J) = 0.29$ for $S = 1/2$, and $\hbar D_s/(a^2 J_{cl}) = 0.33/S$ for $S \to \infty$.

4. Conclusions and open problems

In this paper we have used an analogy between the Kubo formula for disordered electrons and the dynamic spin stiffness tensor of localized quantum spin models to define several new quantities that characterize the dynamic behavior of Heisenberg ferromagnets in the paramagnetic regime. The key observation is that, after proper rescaling, the dynamic spin stiffness tensor of the spin system and the current response kernel of the electronic system can be written in a formally identical way. The proper definition of the Thouless number and the dimensionless conductance in the spin system directly follow from this analogy. As a first application, we have used the Thouless number to develop a simple extrapolation scheme for the calculation of the spin diffusion coefficient at infinite temperatures.

This work opens a number of new directions for further research: A generalization of the concepts developed here to antiferromagnets or Hubbard models seems possible, although some technical difficulties might be encountered. The analogy between electrons in the presence of disorder and spin models in the paramagnetic regime might serve as a useful guide to understand spin diffusion in two dimensions. A Schwinger-Boson calculation of $D_s$ in two-dimensional Heisenberg models at low temperatures has recently been given by Chubukov 16. His result for $D_s$ in ferromagnets can be easily reproduced if we translate the Drude formula for the dimensionless conductance $\tilde{g}_0$ of an electronic system into spin language. By comparing the expressions for the diamagnetic tensors $D_{\mu\nu}$ and $\tilde{D}_{\mu\nu}$ given in Eqs. 4.14 and A.2, we conclude that the energy $\hbar^2 N/(m_e L^2)$ corresponds to $\hbar^2 NS^2/(m_s L^2)$ in the spin model. Here we have used the fact that for $T \ll JS^2$ the spin-correlation length is exponentially large compared with the lattice spacing 17, so that the summation in Eq. A.10 yields $NS^2$. Hence, to obtain the Drude result for $D_s$, we should replace $\hbar^2 N/(m_e L^2) \to \hbar^2 NS^2/(m_s L^2) = JS^2$ in Eq. A.13. This gives for the Thouless
number in the Drude approximation

\[ g_0 = J S^2 \frac{\tau}{\hbar}, \]  

(4.1)

Here \( \tau \) is the characteristic lifetime of single-particle excitations at wavelengths large compared with the spin correlation length. To determine \( \tau \), a microscopic calculation is necessary. Combining Eqs. (1) and (2.19), we conclude that the spin diffusion coefficient in \( d = 2 \) is at low temperatures given by

\[ \hbar D_s a^{-2} = \frac{JS^2 \tau}{\chi \hbar}, \]  

(4.2)

Eq. (4.2) agrees exactly with the result of Chubukov, who performed a diagrammatic calculation within the Schwinger-Boson formalism. The factor of \( JS^2 \) in the numerator is interpreted by Chubukov as transport coefficient. Note, however, that in \( d = 2 \) the Thouless number for non-interacting electrons in the presence of disorder scales to zero in the thermodynamic limit, so that the system is an insulator. Assuming that our analogy can also be applied to this case, we speculate that for any \( T > 0 \) the two-dimensional Heisenberg model corresponds to an insulator, so that the spin diffusion coefficient vanishes. In any case, we expect that in two dimensions the interaction between the diffusion modes will be very important, so that the Drude result given in Eq. (4.2) cannot be trusted. Non-perturbative methods are necessary to understand spin diffusion in the low temperature regime of two dimensional Heisenberg models.

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In this appendix we shall rewrite the standard Kubo formula for the conductivity of an electronic system in a rescaled form. By comparing the rescaled form of the current-response kernel $\tilde{K}_{\mu\nu}$ with the spin stiffness tensor $K_{ij}^{\mu\nu}$ defined in Sec., the proper definition of the Thouless number and the dimensionless spin conductance become obvious. Except for a tilde, we shall use the same symbols as in the spin problem to emphasize the close similarity between the rescaled current-response kernel and spin stiffness tensor.

Consider a $d$-dimensional box of volume $L^d$ containing $N$ electrons with mass $m_e$. Within linear response theory, the change in the current density $\delta j_{\mu}(r, t)$ due to a change in the vector potential $\delta A_{\nu}(r', t')$ is given by

$$\delta j_{\mu}(r, t) = (\alpha L^{2-d}/\hbar) \int_{-\infty}^{\infty} dt' \int d^d r' \sum_{\nu} \tilde{K}_{\mu\nu}(r, r', t-t') \delta A_{\nu}(r', t') , \quad (A.1)$$

where $\alpha = e^2/(\hbar c) \approx 1/137$ is the fine-structure constant. For reasons obvious below, we have not included the factor $\alpha L^{2-d}/\hbar$ into the definition of $\tilde{K}_{\mu\nu}$. The Kubo formula for the Fourier transform of the current response kernel yields

$$\tilde{K}_{\mu\nu}(k, E) = \tilde{D}_{\mu\nu} + \tilde{P}_{\mu\nu}(k, E),$$

where the diamagnetic- and paramagnetic parts are given by

$$\tilde{D}_{\mu\nu} = -\delta_{\mu\nu} \frac{\hbar^2}{m_e L^2} N , \quad (A.2)$$

$$\tilde{P}_{\mu\nu}(k, E) = \sum_{n,m} p_n \left[ \frac{<n|\tilde{J}_{\mu}(k)|m> <m|\tilde{J}_{\nu}(-k)|n>} {E_m - E_n - E} 
 + \frac{<n|\tilde{J}_{\nu}(k)|m> <m|\tilde{J}_{\mu}(-k)|n>} {E_m - E_n + E} \right] , \quad (A.3)$$

and the current operators $\tilde{J}_{\mu}(k)$ are defined by

$$\tilde{J}_{\mu}(k) = \frac{\hbar^2}{m_e L} \int d^d r e^{ik \cdot r} \frac{1}{2i} \left[ \hat{\psi}^\dagger(r) \frac{\partial}{\partial x^\mu} \hat{\psi}(r) - h.c. \right] , \quad (A.4)$$

Here $\hat{\psi}(r)$ is the usual second quantized field operator for the electrons. Note that with this rescaling the $\tilde{J}_{\mu}$ has units of energy, just like the spin currents defined in Eq.1.8. The dimensionless conductance $\tilde{g}(\omega) = L^{d-2} \sigma(\omega)/(e^2/\hbar)$, and the (rescaled) London kernel $\tilde{K}_{xy}(k)$ are given by

$$\tilde{g}(\omega) = \lim_{k \to 0} \frac{\tilde{K}_{11}(k, \hbar \omega + i0^+)}{\hbar (\hbar \omega + i0^+)} \quad (A.5)$$
\[ \tilde{K}^s(k) = - \lim_{\omega \to 0} \tilde{K}_{11}(k, \hbar \omega + i0^+) . \quad (A.6) \]

From Eq. (A.5) it is clear that the factor \( \alpha L^2 / \hbar \) in Eq. (A.1) is very natural. Note that the "\( \omega \)-limit" (where the limit \( \omega \to 0 \) is taken after the limit \( k \to 0 \)) and the "\( k \)-limit" (where the limit \( k \to 0 \) is taken after the limit \( \omega \to 0 \)) describe very different physical properties of the system. The energy \( \tilde{K}_0^s = \lim_{k \to 0} \tilde{K}^s(k) \) is proportional to the density of superconducting electrons. Comparing of Eqs. (1.9) and Eqs. (A.6), it is evident that \( L^2 / \hbar \tilde{K}_0^s \) corresponds to \( \rho_s^0 \) in the spin system. Both quantities are only finite in the presence of off-diagonal long-range order. From Eq. (A.5) we obtain

\[ \text{Re}\tilde{g}(\omega) = \pi \tilde{K}_0 \delta(\hbar \omega) + \tilde{P}(\omega) , \quad \text{Im}\tilde{g}(\omega) = \frac{\tilde{K}(\omega)}{\hbar \omega} , \quad (A.7) \]

with

\[ \tilde{P}(\omega) = \lim_{k \to 0} \frac{\text{Im}\tilde{K}_{11}(k, \hbar \omega + i0^+)}{\hbar \omega} , \quad (A.8) \]

\[ \tilde{K}(\omega) = - \lim_{k \to 0} \text{Re}\tilde{K}_{11}(k, \hbar \omega + i0^+) , \quad (A.9) \]

and \( \tilde{K}_0 = \lim_{\omega \to 0} \tilde{K}(\omega) \). It is instructive to evaluate the above quantities in the simplest possible approximation, where all scattering processes are taken into account by introducing a phenomenological lifetime \( \tau \) in the electronic Greens functions.

At temperatures small compared with the Fermi energy, this yields the well known Drude results\(^{19}\)

\[ \tilde{g}(\omega) = \frac{\hbar N}{m_e L^2} \frac{\tau}{1 - i\omega \tau} , \quad (A.10) \]

\[ \tilde{P}(\omega) = \frac{\hbar N}{m_e L^2} \frac{\tau}{1 + (\omega \tau)^2} , \quad (A.11) \]

\[ \tilde{K}(\omega) = \frac{\hbar^2 N}{m_e L^2} \left[ 1 - \frac{1}{1 + (\omega \tau)^2} \right] . \quad (A.12) \]

The Thouless number \( \tilde{g}_0 \) defined in Eq. (1.2) is in this approximation given by

\[ \tilde{g}_0 = \frac{\hbar N \tau}{m_e L^2} . \quad (A.13) \]

Combining Eqs. (1.2) and (A.13), and using the fact that the level spacing at the Fermi energy in \( d \) dimensions can be expressed in terms of the Fermi velocity \( v_F \) as \( \tilde{\Delta} = m_e v_F^2 / (dN) \), we obtain the classical result for the diffusion coefficient \( D = v_F^2 \tau / d \).