СООБЩЕНИЯ
ОБЪЕДИНЕННОГО
ИНСТИТУТА
ЯДЕРНЫХ
ИССЛЕДОВАНИЙ
ДУБНА

E17 - 12121

E.Kolley, W.Kolley

REMARKS ON THE MAGNON ENERGY IN HUBBARD FERROMAGNETS

1978

E17 - 12121

E.Kolley, W.Kolley

REMARKS ON THE MAGNON ENERGY IN HUBBARD FERROMAGNETS

Коллей Е., Коллей В. E17 - 12121

Об энергии магнонов в хаббардовских ферромагнетиках

Перенормированная магнонная энергия узкозонных ферромагнетиков (при T = 0) получена из полюса восприимчивости, что позволило избежать простой замены затравочного внутриатомного хаббардовского взаимодействия на эффективное. Использовано тождество Уорда для решения уравнения Бете-Солпитера с учетом локального обмена и электрон-электронного лестничного приближения. С помощью неравенства Боголюбова найдены оценка снизу зависящей от волнового вектора поперечной статической восприимчивости и оценка сверху для спинволновой жесткости. Приведен численный пример.

Работа выполнена в Лаборатории теоретической физики ОИЯИ.

Сообщение Объединенного института ядерных исследований. Дубна 1978

Kolley E., Kolley W. E17 - 12121

Remarks on the Magnon Energy in Hubbard Ferromagnets

A renormalized magnon energy of itinerant-electron ferromagnets at zero temperature is calculated by a susceptibility pole ansatz which avoids to replace heuristically the bare intraatomic Hubbard interaction by an effective one. The validity of the Ward identity is stressed in solving the Bethe-Salpeter equation in the presence of local exchange and electron-electron ladders. Bogolubov's inequality is used to derive a lower bound for the momentum-dependent static transverse susceptibility and an upper bound for the spin wave stiffness constant. A numerical example is given.

The investigation has been performed at the Laboratory of Theoretical Physics, JINR.

Communication of the Joint Institute for Nuclear Research. Dubna 1978

1. INTRODUCTION

In a previous study /1/ the magnon energy $\omega_q = Dq^2$ (small momentum q, cubic crystals) for ferromagnetic transition metals was renormalized by taking into account electron-electron correlations on the basis of the Hubbard model /2/

$$H = \sum_{\vec{k}\sigma} \varepsilon_{\vec{k}} n_{\vec{k}\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} . \tag{1}$$

Here $n_{\vec{k}\sigma}$ ($n_{i\sigma}$) is the occupation number operator for Bloch (Wannier) states with spin σ, $\varepsilon_{\vec{k}}$ is the band energy, and U denotes the initial Coulomb interaction. The spin wave stiffness constant D was evaluated from the formula /3/

$$D = \frac{1}{2\langle S^z \rangle} \left[\lim_{q\to 0} \frac{1}{q^2} \langle [S^+_{\vec{q}}, qJ^-_{-\vec{q}}] \rangle - \lim_{\omega\to 0} \lim_{q\to 0} \chi^{+-}_J(\vec{q},\omega) \right] , \tag{2}$$

where $\chi^{+-}_J(\vec{q},\omega)$ means the transverse spin current-current susceptibility, and $2\langle S^z \rangle$ is the magnetization per site. For the Hamiltonian (1) the Fourier transforms of the transverse spin density and current operators are defined by

$$S^{+}_{\vec{q}} = \frac{1}{\sqrt{N}} \sum_{\vec{k}} c^{+}_{\vec{k}\uparrow} c_{\vec{k}+\vec{q}\downarrow} , \qquad S^{-}_{-\vec{q}} = (S^{+}_{\vec{q}})^{+} , \tag{3}$$

$$q J^{+}_{\vec{q}} = \frac{1}{\sqrt{N}} \sum_{\vec{k}} (\varepsilon_{\vec{k}+\vec{q}} - \varepsilon_{\vec{k}}) c^{+}_{\vec{k}\uparrow} c_{\vec{k}+\vec{q}\downarrow} , \qquad J^{-}_{-\vec{q}} = (J^{+}_{\vec{q}})^{+} , \tag{4}$$

resp., where $c^{+}_{\vec{k}\sigma}$ creates an electron in the state $|\vec{k}\sigma\rangle$, and N is the number of lattice sites. Since it is customary to determine D through a pole of the transverse spin density-density susceptibility $\chi^{+-}(\vec{q},\omega)$ one has, on the other hand, the prescription /4/

$$D = -\frac{1}{2\langle S^{z}\rangle} \lim_{\omega\to 0} \lim_{q\to 0} \left[\frac{\omega^{2}}{q^{2}} \left(\chi^{+-}(\vec{q},\omega) + \frac{2\langle S^{z}\rangle}{\omega} \right) \right] . \tag{5}$$

In this paper we calculate the stiffness constant from (5), unlike the approach /1/, by solving a Bethe-Salpeter equation within the local exchange approximation. The resultant D, including particle-particle scatterings by the local ladder approximation (LLA) /5/, coincides with D found in /1/ on the basis of (2). A lower bound for the static susceptibility $\chi^{+-}(\vec{q},\omega=0)$ and, therefore, an upper bound for D are obtained by applying Bogolubov's inequality /6/ (general bound considerations in /7/ were based on the Hohenberg-Kohn theorem). Correlation effects on D and the effective interaction are illustrated by a numerical example.

2. DERIVATION OF D BY SOLVING A BETHE-SALPETER EQUATION

To handle the electron-electron interaction in the framework of the perturbation theory the transverse susceptibilities in (2) and (5) must be formulated within a microscopic Fermi liquid approach /4/. Hence, at zero temperature, the following expressions in terms of causal functions can be written down:

$$\begin{aligned} \chi^{+-}(\vec{q},\omega) &= -\langle\langle S^{+}_{\vec{q}}, S^{-}_{-\vec{q}} \rangle\rangle_{\omega} = i \int dt\, e^{i\omega t} \langle T S^{+}_{\vec{q}}(t) S^{-}_{-\vec{q}}(0) \rangle \\ &= \frac{i}{N} \int \frac{dE}{2\pi} \sum_{\vec{k}} G_{\vec{k}\uparrow}(E) \Lambda_{0-\vec{q}\uparrow\downarrow}(E,E+\omega) G_{\vec{k}+\vec{q}\downarrow}(E+\omega) , \end{aligned} \tag{6}$$

$$\begin{aligned} \chi^{+-}_{1}(\vec{q},\omega) &= -\langle\langle q J^{+}_{\vec{q}}, S^{-}_{-\vec{q}} \rangle\rangle_{\omega} = \frac{i}{N} \int \frac{dE}{2\pi} \sum_{\vec{k}} G_{\vec{k}\uparrow}(E) \Lambda_{1\vec{k}\uparrow\vec{k}+\vec{q}\downarrow}(E,E+\omega) G_{\vec{k}+\vec{q}\downarrow}(E+\omega) \\ &= -\langle\langle S^{+}_{\vec{q}}, q J^{-}_{-\vec{q}} \rangle\rangle_{\omega} = \frac{i}{N} \int \frac{dE}{2\pi} \sum_{\vec{k}} (\varepsilon_{\vec{k}+\vec{q}} - \varepsilon_{\vec{k}}) G_{\vec{k}\uparrow}(E) \Lambda_{0-\vec{q}\uparrow\downarrow}(E,E+\omega) G_{\vec{k}+\vec{q}\downarrow}(E+\omega) , \end{aligned} \tag{7}$$

$$q^{2} \chi^{+-}_{J}(\vec{q},\omega) = -\langle\langle q J^{+}_{\vec{q}}, q J^{-}_{-\vec{q}} \rangle\rangle_{\omega} = \frac{i}{N} \int \frac{dE}{2\pi} \sum_{\vec{k}} (\varepsilon_{\vec{k}+\vec{q}} - \varepsilon_{\vec{k}}) G_{\vec{k}\uparrow}(E) \Lambda_{1\vec{k}\uparrow\vec{k}+\vec{q}\downarrow}(E,E+\omega) G_{\vec{k}+\vec{q}\downarrow}(E+\omega) , \tag{8}$$

where $\langle\ldots\rangle$ means the ground-state expectation value, $G_{\vec{k}\sigma}(E)$ denotes the one-particle Green function, and $\chi^{+-}_{1}(\vec{q},\omega)$ is the transverse spin current-density susceptibility. The effective spin-flip vertices $\Lambda_{0-\vec{q}\uparrow\downarrow}$ and $\Lambda_{1\vec{k}\uparrow\vec{k}+\vec{q}\downarrow}$ satisfy the Bethe-Salpeter-type equations

$$\Lambda_{0-\vec{q}\uparrow\downarrow}(E,E+\omega) = 1 - \int \frac{d\bar{E}}{2\pi} i I_{\uparrow\downarrow\downarrow\uparrow}(E,\bar{E}+\omega;\omega) \frac{1}{N} \sum_{\vec{k}} G_{\vec{k}\uparrow}(\bar{E}) \Lambda_{0-\vec{q}\uparrow\downarrow}(\bar{E},\bar{E}+\omega) G_{\vec{k}+\vec{q}\downarrow}(\bar{E}+\omega) , \tag{9}$$

$$\Lambda_{1\vec{k}\uparrow\vec{k}+\vec{q}\downarrow}(E,E+\omega) = \varepsilon_{\vec{k}+\vec{q}} - \varepsilon_{\vec{k}} - \int \frac{d\bar{E}}{2\pi} i I_{\uparrow\downarrow\downarrow\uparrow}(E,\bar{E}+\omega;\omega) \frac{1}{N} \sum_{\vec{k}'} G_{\vec{k}'\uparrow}(\bar{E}) \Lambda_{1\vec{k}'\uparrow\vec{k}'+\vec{q}\downarrow}(\bar{E},\bar{E}+\omega) G_{\vec{k}'+\vec{q}\downarrow}(\bar{E}+\omega) , \tag{10}$$

where the irreducible particle-hole vertex $I_{\uparrow\downarrow\downarrow\uparrow}(E,\bar{E}+\omega\,;\omega)\equiv I_{\uparrow\downarrow\downarrow\uparrow}(E,$ $\bar{E}+\omega\,;E+\omega\,,\bar{E})$, presumed to be site-diagonal, mediates the local exchange.

In the particle-particle channel we make use of the LLA scheme /5/

$$\Sigma_\sigma(E)=\int\frac{d\bar{E}}{2\pi i}G_{-\sigma}(\bar{E})T(E+\bar{E}), \tag{11}$$

$$T(E)=\left[\frac{1}{U}+\int\frac{d\bar{E}}{2\pi i}G_\sigma(\bar{E})G_{-\sigma}(E-\bar{E})\right]^{-1}, \tag{12}$$

$$n=\sum_\sigma n_\sigma=\sum_\sigma\int\frac{dE}{2\pi i}G_\sigma(E)\,;\qquad G_\sigma(E)=\frac{1}{N}\sum_{\vec{k}}G_{\vec{k}\sigma}(E), \tag{13}$$

$$G^{-1}_{\vec{k}\sigma}(E)=E-\varepsilon_{\vec{k}}-\Sigma_\sigma(E), \tag{14}$$

where $\Sigma_\sigma(E)$ is the self-energy, $T(E+\bar{E})$ denotes the two-particle vertex, and n (n_σ) is the average number of electrons per site (with spin σ). In the particle-hole channel we choose the kernel

$$I_{\uparrow\downarrow\downarrow\uparrow}(E,\bar{E}+\omega;\omega)=-T(E+\bar{E}+\omega). \tag{15}$$

By substituting (15) into (9) and (10), using (11) and the dressed propagator (14) one proves, for the present approximation, the validity of the Ward-Takahashi-relation (cf.,e.g., /8/)

$$\omega\Lambda_{0-\vec{q}\uparrow\downarrow}(E,E+\omega)-\Lambda_{1\vec{k}\vec{k}+\vec{q}\atop\uparrow\;\;\downarrow}(E,E+\omega)=G^{-1}_{\vec{k}+\vec{q}\downarrow}(E+\omega)-G^{-1}_{\vec{k}\uparrow}(E). \tag{16}$$

The Ward identity (16) leads together with (6) and (7) to

$$\omega\chi^{+-}(\vec{q},\omega)-\chi^{+-}_1(\vec{q},\omega)=n_\downarrow-n_\uparrow=-2\langle S^z\rangle. \tag{17}$$

Furthermore, on combining (7), (8), and (16) one gets

$$\begin{aligned}\omega\chi^{+-}_1(\vec{q},\omega)-q^2\chi^{+-}_J(\vec{q},\omega)&=-C_{\vec{q}}\\&=\frac{i}{N}\int\frac{dE}{2\pi}\sum_{\vec{k}}\left[(\varepsilon_{\vec{k}+\vec{q}}-\varepsilon_{\vec{k}})G_{\vec{k}\uparrow}(E)+(\varepsilon_{\vec{k}-\vec{q}}-\varepsilon_{\vec{k}})G_{\vec{k}\downarrow}(E)\right].\end{aligned} \tag{18}$$

Note that (17) and (18) hold rigorously (without approximations) as can be shown immediately from the equations of motion.

In order to solve the integral equation (9) via (15) we replace $T(E+\bar{E}+\omega)$ by an approximated kernel $\tilde{T}(E,E+\omega)$, yielding with (6) the relation

$$\Lambda_{0-\vec{q}\uparrow\downarrow}(E,E+\omega)=1+\tilde{T}(E,E+\omega)\chi^{+-}(\vec{q},\omega). \tag{19}$$

Analogously, from (10) and (7) it follows that

$$\Lambda_{1\vec{k}\vec{k}+\vec{q}\atop\uparrow\;\;\downarrow}(E,E+\omega)=\varepsilon_{\vec{k}+\vec{q}}-\varepsilon_{\vec{k}}+\tilde{T}(E,E+\omega)\chi^{+-}_1(\vec{q},\omega). \tag{20}$$

To determine $\tilde{T}(E,E+\omega)$ explicitly one has to fulfil the Ward identity (16). By inserting (19) and (20) into (16), provided that the r.h.s. of (16) is expressed by (14), we find

$$\tilde{T}(E,E+\omega)=\frac{\Sigma_\uparrow(E)-\Sigma_\downarrow(E+\omega)}{n_\downarrow-n_\uparrow}, \tag{21}$$

where (17) was used, too. Now one substitutes (19) into (6), and (20) into (7) to obtain the solutions

$$\chi^{+-}(\vec{q},\omega) = \frac{\hat{\chi}_0(\vec{q},\omega)}{1-\tilde{\chi}(\vec{q},\omega)}, \qquad (22)$$

$$\chi_1^{+-}(\vec{q},\omega) = \frac{\hat{\chi}_1(\vec{q},\omega)}{1-\tilde{\chi}(\vec{q},\omega)} \qquad (23)$$

with the abbreviations

$$\hat{\chi}_0(\vec{q},\omega) = \frac{i}{N}\int\frac{dE}{2\pi}\sum_{\vec{k}} G_{\vec{k}\uparrow}(E)G_{\vec{k}+\vec{q}\downarrow}(E+\omega), \qquad (24)$$

$$\hat{\chi}_1(\vec{q},\omega) = \frac{i}{N}\int\frac{dE}{2\pi}\sum_{\vec{k}} G_{\vec{k}\uparrow}(E)G_{\vec{k}+\vec{q}\downarrow}(E+\omega)\,(\varepsilon_{\vec{k}+\vec{q}}-\varepsilon_{\vec{k}}), \qquad (25)$$

$$\tilde{\chi}(\vec{q},\omega) = \frac{i}{N}\int\frac{dE}{2\pi}\sum_{\vec{k}} G_{\vec{k}\uparrow}(E)G_{\vec{k}+\vec{q}\downarrow}(E+\omega)\tilde{T}(E,E+\omega). \qquad (26)$$

On the other hand, the time-reversal symmetry involved in (7) leads on the basis of (19) to $\chi_1^{+-}(\vec{q},\omega) = \hat{\chi}_1(\vec{q},\omega) + \tilde{\chi}_1(\vec{q},\omega)\,\chi^{+-}(\vec{q},\omega)$, implying in view of (22) and (23) the condition

$$\hat{\chi}_0(\vec{q},\omega)\,\tilde{\chi}_1(\vec{q},\omega) = \hat{\chi}_1(\vec{q},\omega)\,\tilde{\chi}(\vec{q},\omega), \qquad (27)$$

where

$$\tilde{\chi}_1(\vec{q},\omega) = \frac{i}{N}\int\frac{dE}{2\pi}\sum_{\vec{k}} G_{\vec{k}\uparrow}(E)G_{\vec{k}+\vec{q}\downarrow}(E+\omega)\tilde{T}(E,E+\omega)\,(\varepsilon_{\vec{k}+\vec{q}}-\varepsilon_{\vec{k}}). \qquad (28)$$

It is pointed out that (27) is fulfilled trivially in two cases: at $\vec{q}=0$ and in the Hartree-Fock approximation $\Sigma_\sigma = Un_{-\sigma}$, where (21) is reduced to $\tilde{T}=U$.

On combining (22) and (23) with (17) the pole in (22) can be rewritten as $\chi^{+-}(\vec{q},\omega) = (n_\downarrow - n_\uparrow)\left[\omega - \frac{\hat{\chi}_1(\vec{q},\omega)}{\hat{\chi}_0(\vec{q},\omega)}\right]^{-1}$ which has to obey the necessary and sufficient condition (27), i.e.,

$$\chi^{+-}(\vec{q},\omega) = \frac{n_\downarrow - n_\uparrow}{\omega - \dfrac{\tilde{\chi}_1(\vec{q},\omega)}{\tilde{\chi}(\vec{q},\omega)}}. \qquad (29)$$

The calculation of low-lying spin wave excitations requires expanding (28) to second order in $\vec{q}$:

$$\tilde{\chi}_1(\vec{q},\omega) = \frac{i}{2N}\int\frac{dE}{2\pi}\sum_{\vec{k}} G_{\vec{k}\uparrow}(E)G_{\vec{k}\downarrow}(E+\omega)\left[G_{\vec{k}\downarrow}(E+\omega)-G_{\vec{k}\uparrow}(E)\right]\tilde{T}(E,E+\omega)(\vec{q}\cdot\nabla_{\vec{k}}\varepsilon_{\vec{k}})^2, \qquad (30)$$

where

$$G_{\vec{k}\uparrow}(E)G_{\vec{k}\downarrow}(E+\omega) = \frac{G_{\vec{k}\uparrow}(E) - G_{\vec{k}\downarrow}(E+\omega)}{\omega - \Sigma_\downarrow(E+\omega) + \Sigma_\uparrow(E)} \qquad (31)$$

which results from (14). Define the magnon energy in the denominator of (29) by $Dq^2 = \left.\frac{\tilde{\chi}_1(\vec{q},\omega)}{\tilde{\chi}(\vec{q},\omega)}\right|_{\omega=0}$ or, equivalently, D according to (5). First, one gets from (26) by using (21) and (31) the static limit $\tilde{\chi}(\vec{q}=0,\omega=0)=1$. Secondly, to order q^2, $\tilde{\chi}_1(\vec{q},\omega=0)$ is available from (30) to derive by means of (21) and (31) the spin wave stiffness constant

$$D = \frac{1}{6(n_\uparrow - n_\downarrow)}\frac{i}{N}\int\frac{dE}{2\pi}\sum_{\vec{k}}\left[G_{\vec{k}\uparrow}(E)-G_{\vec{k}\downarrow}(E)\right]^2(\nabla_{\vec{k}}\varepsilon_{\vec{k}})^2, \qquad (32)$$

where cubic symmetry was employed. Going over to retarded („r") Green functions we obtain

$$D = \frac{1}{6\pi(n_\uparrow - n_\downarrow)}\,\mathrm{Im}\int_{-\infty}^{\mu} dE\,\frac{1}{N}\sum_{\vec{k}}\left[G^r_{\vec{k}\uparrow}(E)-G^r_{\vec{k}\downarrow}(E)\right]^2(\nabla_{\vec{k}}\varepsilon_{\vec{k}})^2, \qquad (33)$$

where μ denotes the Fermi level. The expression (33) agrees with the result for D obtained in /1/. Additional vertex corrections to the stiffness formula do not appear. These are cancelled by the Ward identity (16) and the symmetry relation (27), leaving just the propagator renormalization. The pole behaviour of $\chi^{+-}(\vec{q},\omega)$ is here explicitly derived unlike the treatment /1/. Especially, the present scheme makes evident the influence of electron-electron ladders on the particle-hole channel.

3. BOUNDS ON $\chi^{+-}(\vec{q},\omega=0)$ AND D

As has been shown in section 2, D is directly related to the inverse of the static transverse susceptibility $\chi^{+-}(\vec{q},\omega=0)$. Thus it is useful to consider Bogolubov's inequality /6/

$$|\langle\langle A,B\rangle\rangle_{\omega=0}|^2 \leq |\langle\langle A,A^+\rangle\rangle_{\omega=0}||\langle\langle B^+,B\rangle\rangle_{\omega=0}| \tag{34}$$

or, equivalently (cf. /9/),

$$|\langle[Q,B]\rangle|^2 \leq |\langle[Q,[Q^+,H]]\rangle||\langle\langle B^+,B\rangle\rangle_{\omega=0}| . \tag{35}$$

Bogolubov's inequality was applied in /10,11/ to itinerant-electron systems to prove the absence of magnetic ordering in one and two dimensions at nonzero temperature.

In this section we estimate the magnon energy of Hubbard ferromagnets at zero temperature. Choosing $B_{\vec{q}}=S^-_{-\vec{q}}$ and $A_{\vec{q}}=qJ^+_{\vec{q}}$ defined in (3) and (4) we write (34) in the form

$$\frac{4\langle S^z\rangle^2}{|\langle\langle qJ^+_{\vec{q}},qJ^-_{-\vec{q}}\rangle\rangle_{\omega=0}|} \leq |\langle\langle S^+_{\vec{q}},S^-_{-\vec{q}}\rangle\rangle_{\omega=0}|, \tag{36}$$

where $\langle\langle qJ^+_{\vec{q}},S^-_{-\vec{q}}\rangle\rangle_{\omega=0} = -\langle[S^+_{\vec{q}},S^-_{-\vec{q}}]\rangle = -2\langle S^z\rangle$ was used as a consequence of (17) combined with (7). On the other hand, one can express (35) with $Q_{\vec{q}}=S^+_{\vec{q}}$, $B_{\vec{q}}=S^-_{-\vec{q}}$, and H from (1) as

$$\frac{4\langle S^z\rangle^2}{|C_{\vec{q}}|} \leq |\langle\langle S^+_{\vec{q}},S^-_{-\vec{q}}\rangle\rangle_{\omega=0}|, \tag{37}$$

which also follows directly from (36) by taking the limit $\omega\to 0$ in (18) together with (8). From (18) $C_{\vec{q}}$ becomes

$$C_{\vec{q}} = \frac{1}{N}\sum_{ij} t_{ij}\left\{(e^{-i\vec{q}(\vec{R}_i-\vec{R}_j)}-1)\langle c^+_{i\uparrow}c_{j\uparrow}\rangle + (e^{i\vec{q}(\vec{R}_i-\vec{R}_j)}-1)\langle c^+_{i\downarrow}c_{j\downarrow}\rangle\right\}, \tag{38}$$

where $c^+_{i\sigma}$ ($c_{i\sigma}$) creates (annihilates) a spin σ electron in the Wannier state at lattice site i, $t_{ij}=\frac{1}{N}\sum_{\vec{k}}\varepsilon_{\vec{k}}\, e^{i\vec{k}(\vec{R}_i-\vec{R}_j)}$ are the hopping integrals, and $\vec{R}_i$ is the position vector of site i.

Dealing with long wavelength excitations we quote $C_{\vec{q}}$ in the lowest order of $\vec{q}$, i.e., in order q^2. It is

$$C_{\vec{q}} = -\frac{q^2}{6N}\sum_{ij\sigma} t_{ij}(\vec{R}_i-\vec{R}_j)^2\langle c^+_{i\sigma}c_{j\sigma}\rangle, \tag{39}$$

where cubic symmetry is presumed. An estimation of $C_{\vec{q}}$ is performed by restricting to a sc lattice and including only nearest-neighbour hopping integrals $t_{ij}=t$. Then one may write

$$|C_{\vec{q}}| = \frac{q^2a^2t}{6N}\left|\sum_{i\sigma}\sum_{j(\neq i)}{}'\langle c^+_{i\sigma}c_{j\sigma}\rangle\right| \leq q^2a^2tn, \tag{40}$$

where $|\langle c_{i\sigma}^{+} c_{j\sigma}\rangle| \leq n_{\sigma}$ is used, and a is the lattice constant. Substitution of (40) into (37) gives a lower bound for the static transverse susceptibility

$$\frac{(n_{\uparrow}-n_{\downarrow})^2}{n a^2 t}\frac{1}{q^2} \leq |\langle\langle S_{\vec{q}}^{+}, S_{-\vec{q}}^{-}\rangle\rangle_{\omega=0}| = |\chi^{+-}(\vec{q},\omega=0)|. \tag{41}$$

This implies (cf. the context of (29)) an upper bound for the stiffness constant

$$D \leq a^2 t \tag{42}$$

which is written down in the saturated ferromagnetic case.

Additionally, we introduce the spectral decomposition /6/

$$\chi^{+-r}(\vec{q},\omega) = -\langle\langle S_{\vec{q}}^{+}, S_{-\vec{q}}^{-}\rangle\rangle_{\omega}^{+} = -\frac{1}{2\pi}\int_{-\infty}^{\infty} d\omega' \frac{\operatorname{sign}\omega'}{\omega-\omega'+i\varepsilon} I_{S_{\vec{q}}^{+}S_{-\vec{q}}^{-}}(\omega'), \tag{43}$$

where $I_{S_{\vec{q}}^{+}S_{-\vec{q}}^{-}}(\omega) \geq 0$ is the spectral density at zero temperature. The static susceptibility becomes

$$-\langle\langle S_{\vec{q}}^{+}, S_{-\vec{q}}^{-}\rangle\rangle_{\omega=0} = \frac{1}{2\pi}\int_{-\infty}^{\infty} d\omega' \frac{1}{|\omega'|} I_{S_{\vec{q}}^{+}S_{-\vec{q}}^{-}}(\omega') > 0. \tag{44}$$

Let us define the mean excitation spectrum by the moments (cf. /12,13/)

$$\overline{\omega_{\vec{q}}^{n}} = \frac{\int_{0}^{\infty}\frac{d\omega}{2\pi}\,\omega^{n-1}\left(I_{S_{\vec{q}}^{+}S_{-\vec{q}}^{-}}(\omega) + I_{S_{-\vec{q}}^{-}S_{\vec{q}}^{+}}(\omega)\right)}{\int_{0}^{\infty}\frac{d\omega}{2\pi}\,\frac{1}{\omega}\left(I_{S_{\vec{q}}^{+}S_{-\vec{q}}^{-}}(\omega) + I_{S_{-\vec{q}}^{-}S_{\vec{q}}^{+}}(\omega)\right)}, \quad (n=1,2,\ldots). \tag{45}$$

Then one verifies the average energy of the excitations to be

$$\overline{\omega_{\vec{q}}} = \frac{\zeta_{\vec{q}}}{-\langle\langle S_{\vec{q}}^{+}, S_{-\vec{q}}^{-}\rangle\rangle_{\omega=0}}, \tag{46}$$

where

$$\zeta_{\vec{q}} = \int_{-\infty}^{\infty}\frac{d\omega}{2\pi} I_{S_{\vec{q}}^{+}S_{-\vec{q}}^{-}}(\omega) = \langle S_{\vec{q}}^{+}S_{-\vec{q}}^{-} + S_{-\vec{q}}^{-}S_{\vec{q}}^{+}\rangle > 0. \tag{47}$$

Here we have used $I_{S_{\vec{q}}^{+}S_{-\vec{q}}^{-}}(\omega) = I_{S_{-\vec{q}}^{-}S_{\vec{q}}^{+}}(-\omega)$ to replace the denominator of (45) by (44). Note that (47) is to be distinguished from the sum rule $\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\operatorname{sign}\omega\, I_{S_{\vec{q}}^{+}S_{-\vec{q}}^{-}}(\omega) = 2\langle S^{z}\rangle$. The second moment yields

$$\overline{\omega_{\vec{q}}^{2}} = \frac{C_{\vec{q}}}{-\langle\langle S_{\vec{q}}^{+}, S_{-\vec{q}}^{-}\rangle\rangle_{\omega=0}} = \frac{\langle\langle qJ_{\vec{q}}^{+}, qJ_{-\vec{q}}^{-}\rangle\rangle_{\omega=0}}{\langle\langle S_{\vec{q}}^{+}, S_{-\vec{q}}^{-}\rangle\rangle_{\omega=0}}, \tag{48}$$

where $\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\,\omega\operatorname{sign}\omega\, I_{S_{-\vec{q}}^{-}S_{\vec{q}}^{+}}(\omega) = -\langle[S_{\vec{q}}^{+},[S_{-\vec{q}}^{-},H]]\rangle$ (f-sum rule) was employed. The relation $\omega^2 I_{S_{\vec{q}}^{+}S_{-\vec{q}}^{-}}(\omega) = I_{qJ_{\vec{q}}^{+}qJ_{-\vec{q}}^{-}}(\omega)$ can also be chosen to get (48); compare (18) at $\omega=0$ and $\vec{q}\neq 0$. Note that $-\langle\langle qJ_{\vec{q}}^{+}, qJ_{-\vec{q}}^{-}\rangle\rangle_{\omega=0} \geq 0$.

Using (37) and (40) we can estimate (46) and (48) as

$$\overline{\omega_{\vec{q}}} \leq \frac{C_{\vec{q}}}{4\langle S^z\rangle^2}\zeta_{\vec{q}} \leq \frac{a^2 t n}{4\langle S^z\rangle^2} q^2 \zeta_{\vec{q}}, \tag{49}$$

$$\overline{\omega_{\vec{q}}^{2}} \leq \frac{C_{\vec{q}}^{2}}{4\langle S^z\rangle^2} \leq \frac{a^4 t^2 n^2}{4\langle S^z\rangle^2} q^4, \tag{50}$$

where the r.h.s. are valid for sufficiently small q. The definition (45) predicts $\overline{\omega_{\vec{q}}^{2}} \geq \overline{\omega_{\vec{q}}}^{2}$ so that $\zeta_{\vec{q}} \leq 2|\langle S^{z}\rangle|$ for $q \to 0$ /12/. Then (49) and (50) refer to the existence of gapless spin wave excitations provided that $\langle S^z \rangle \neq 0$. Putting $\overline{\omega}_{\vec q} \equiv \omega_q = Dq^2$ and going over to the saturated case we arrive again at (42).

4. A NUMERICAL EXAMPLE

To illustrate the use of the formula (32) for D we solve the LLA scheme (11) to (14) self-consistently and compare the results with those of the Hartree-Fock treatment (see Fig.1b). The following assumptions have been made /1/: a sc lattice with a semielliptic unperturbed density of states (bandwidth 2w=12t, in reduced units 2w=1) and the velocity dispersion law $\frac{1}{N}\sum_{\vec k}\delta(E-\varepsilon_{\vec k})(\nabla_{\vec k}\varepsilon_{\vec k})^2 = \frac{2v_m^2}{\pi w}\left(1-\left(\frac{E}{w}\right)^2\right)^{3/2}\theta(w-|E|)$ (v_m is of order wa). In Fig.1a the special value $\Gamma = T(2\mu)$ of the ladder vertex function $T(E+\bar E)$ indicates the renormalization of the bare interaction U. The application of (42) to the present example yields $D/d_o \leq 3/4$ which is fulfilled in both approximations. The tendency of the D-curves refers to the validity of this estimation for larger U, too.

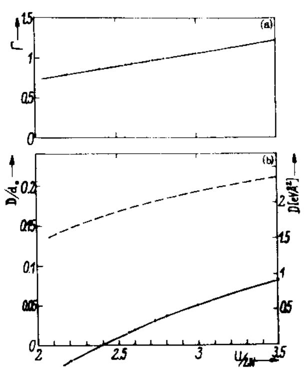

Fig.1.a) Effective Coulomb interaction Γ (in units of the bandwidth 2w) and b) spin wave stiffness constant D vs. bare U/2w for n=0.5. D is scaled in units of $d_o = \frac{2}{9}wa^2$ and in absolute units with 2w=6.3eV, a=4Å; the dashed line shows Hartree-Fock results.

REFERENCES

1. Kolley E., Kolley W. phys.stat.sol.(b), 1978, 90, p.K103.
2. Hubbard J. Proc.Roy.Soc., 1963, A276, p.238.
3. Edwards D.M., Fisher B. J.Physique, 1971, 32, p.C1-697.
4. Kolley E., Kolley W. JINR, E17-11771, Dubna,1978.
5. Babanov Yu.A., Naish V.E., Sokolov O.B., Finashkin V.K. phys. stat.sol.(b), 1973, 56, p.K87.
6. Боголюбов Н.Н. Сб. "Статистическая физика и квантовая теория поля", "Наука", I973, с. 7.
7. Liu K.L., Vosko S.H. J.Phys., 1978, F8, p.1539.
8. Hertz J.A., Edwards D.M. Phys.Rev.Lett., 1972, 28, p.1334; J.Phys., 1973, F3, p.2174.
9. Боголюбов Н.Н. (мл.), Садовников Б.И. Некоторые вопросы статистической механики, "Высш. школа", I975.
10. Wegner F. Phys.Lett., 1967, 24A, p.131.
11. Walker M.B., Ruijgrok Th.W. Phys.Rev., 1968, 171, p.513.
12. Wagner H. Z.Physik, 1966, 195, p.273.
13. Izuyama T. Phys.Rev., 1972, B5, p.190.

Received by Publishing Department
on December 22, 1978.