Generalized Spin Susceptibility in the Narrow-s-Band Model*

J. W. Schweitzer
Department of Physics and Astronomy, The University of Iowa, Iowa City, Iowa 52240

and

Julian D. Maynard, Jr.†
Department of Physics, Princeton University, Princeton, New Jersey 08540
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A calculation of the reduced spin susceptibility $\chi(q, \omega)$ of the paramagnetic phase of a system of electrons described by the narrow-s-band model is presented. The treatment is based on the two-pole approximation for electron correlation in narrow energy bands by Roth. An approximate expression for $\chi(q, \omega)$ in the strongly correlated limit is given. This expression is intended to be a valid approximation for the strongly correlated limit at higher carrier densities where low-density T-matrix results would be inapplicable.

I. INTRODUCTION

This paper presents a derivation of an approximate expression for the reduced generalized spin susceptibility $\chi(q, \omega)$ of the paramagnetic phase of a system of interacting electrons in a narrow s band for the situation in which the electron-electron interaction is large compared with the bandwidth. One is particularly interested in the susceptibility for the interaction large compared with the bandwidth, since it can be used to look for instabilities of the paramagnetic state toward magnetic ordering which is expected for a sufficiently large interaction energy. The previous treatments[1,2] based on the random-phase approximation are inapplicable when the interaction is large; and, except for the low-density limit,[3] approximate methods used to treat this system in the strongly correlated limit are of uncertain validity. A recent calculation of the spin susceptibility by Hubbard and Jain[4] is intended to be a valid approximation for both the limits of the electron-electron interaction small and large compared with the bandwidth. However, their treatment is based on the narrow-energy-band correlation theory of Hubbard[5] which has the apparent failure of yielding the result that the system is never ferromagnetic for a simply shaped density of states regardless of the size of the interaction.

In this paper we base our calculation of the spin susceptibility on the two-pole approximation of Roth.[6] Her approximation is an improved version of the Hubbard theory which gives a ferromagnetic state in the strongly correlated limit for a simply shaped density of states, provided the concentration of carriers is sufficiently large. The approximation does not reduce to the correct low-density result. The calculation of the spin susceptibility in that limit should be based on the Kanamori approximation.[3] However, the instabilities of the paramagnetic state are expected at the higher carrier concentrations where the two-pole approximation of Roth is a significant improvement[7] on the Kanamori theory. Therefore, the spin susceptibility derived in this paper for the strongly correlated limit is expected to be a valid approximate expression for studying the stability of the paramagnetic phase. Results are also applicable to inelastic magnetic neutron scattering.

In Sec. II the model Hamiltonian for the system is introduced and a general equation of motion procedure is described for evaluating the linear response of the system to a wave number and frequency-dependent external magnetic field. The procedure uses a nonequilibrium generalization of the Roth procedure[8] for linearizing many-body equations of motion. This general procedure is applied in Sec. III to the model Hamiltonian within the two-pole approximation. An explicit expression for the reduced susceptibility $\chi(q, \omega)$ is given for the strongly correlated limit.

II. MODEL HAMILTONIAN AND GENERAL PROCEDURE

The Hubbard Hamiltonian[5] for a system of electrons in a narrow s band is

$$H_0 = \sum_{ij\sigma} T_{ij} c^{\dagger}_{i\sigma} c_{j\sigma} + \tfrac{1}{2} I \sum_{i\sigma} n_{i\sigma} n_{i-\sigma}, \tag{1}$$

where I is the interaction energy of two electrons of opposite spin on the same Wannier function and

$$T_{ij} = N^{-1} \sum_k \epsilon_k e^{-i\vec{k}\cdot(\vec{R}_i - \vec{R}_j)} = T_{ji}, \tag{2}$$

the ϵ_k being the one-electron band energies. The R_i labels the atomic sites and N is the number of sites, and the marking of vectors is suppressed in indices and arguments.

In the presence of a varying external magnetic field

$$h_i(t) = \tfrac{1}{2} h_0 e^{-i(\vec{q}\cdot\vec{R} - \omega t)} + \tfrac{1}{2} h_0 e^{i(\vec{q}\cdot\vec{R}_i - \omega t)}, \tag{3}$$

there is a Zeeman interaction

$$H_1 = \tfrac{1}{2} g\mu_B \sum_{i\sigma} h_i(t)\sigma n_{i\sigma}. \tag{4}$$

The generalized reduced susceptibility $\chi(q, \omega)$ describes the linear response of the spins to this field. $\chi(q, \omega)$ is defined by[4]

$$-\tfrac{1}{2} g\mu_B \sum_\sigma \sigma \langle n_{i\sigma}\rangle = \mathrm{Re}[\chi(q, \omega) h_0 e^{i(\vec{q}\cdot\vec{R}_i - \omega t)}], \tag{5}$$

where

$$\langle n_{i\sigma}\rangle \equiv \mathrm{Tr}[\rho(t) n_{i\sigma}]. \tag{6}$$

Here $\rho(t)$ is the density operator, and Eq. (5) is understood in the limit $h_0 \to 0$.

An equation-of-motion technique will be used to study the response of a set of operators $\{A_n(t)\}$ in the Heisenberg representation. In the equation-of-motion method one attempts to find a set of operators $\{A_n\}$ such that

$$[A_n, H] = \sum_m K_{nm} A_m, \tag{7}$$

where H is the Hamiltonian of the system. The eigenvalues of K are then excitation energies of the system. However, for systems with interactions one must in general make approximations. One usually chooses some set $\{A_n\}$, motivated by the apparent important correlations in the system, and approximates $[A_n, H]$ by an expression of the form of Eq. (7) where the matrix K is specified by some prescription. In our treatment we shall use a prescription due to Roth[8] which determines K self-consistently. This prescription will be discussed later in this section.

For a system subject to a perturbation H_1 we have

$$[A_n, H_0 + H_1] \simeq \sum_m K_{nm} A_m \tag{8}$$

and

$$[A_n, H_0] \simeq \sum_m K^0_{nm} A_m(t), \tag{9}$$

where these equations are approximations as previously described. The approximate equations of motion are then

$$i\frac{d}{dt} A_n(t) \simeq \sum_m K_{nm} A_m(t) \tag{10}$$

and

$$i\frac{d}{dt} A^0_n(t) \simeq \sum_m K^0_{nm} A^0_m(t). \tag{11}$$

The zero superscript denotes the Heisenberg operator in the absence of the perturbation. Since we are interested only in the linear response, terms of second order in the perturbation will be neglected. Therefore,

$$i\frac{d}{dt}[A_n(t) - A^0_n(t)] \simeq \sum_m K^0_{nm}[A_m(t) - A^0_m(t)] + \sum_m K^1_{nm} A^0_m(t), \tag{12}$$

where K^1_{nm} is the first-order difference between K_{nm} and K^0_{nm}. Furthermore, for H_1 of the form of Eq. (4) with $h_i(t)$ given by Eq. (3), we make the ansatz

$$K^1_{nm} = K^{(+)}_{nm} e^{i\omega t} + K^{(-)}_{nm} e^{-i\omega t}. \tag{13}$$

A formal solution of Eq. (10) can be easily obtained in terms of the solution of the unperturbed system. Let us define a matrix Q such that

$$\sum_{rs} Q_{nr} K^0_{rs} Q^{-1}_{sm} = E_n \delta_{nm}. \tag{14}$$

The E_n are approximate excitation energies for the system described by H_0. Using Eqs. (11) and (12), we find to first order in the applied field

$$A_n(t) = \sum_r Q^{-1}_{nr}\left[e^{-iE_r t} B_r + \sum_m \left(\frac{\tilde{K}^{(-)}_{rm} e^{-i(E_m+\omega)t}}{\omega + E_m - E_r + i\eta} + \frac{\tilde{K}^{(+)}_{rm} e^{-i(E_m-\omega)t}}{-\omega + E_m - E_r + i\eta}\right) B_m\right]. \tag{15}$$

Here one has the following definitions:

$$B_n = \sum_m Q_{nm} A_m, \tag{16}$$

$$\tilde{K}^{(\pm)} = Q K^{(\pm)} Q^{-1}. \tag{17}$$

The $\eta (\eta \to 0^+)$ describes the external field being adiabatically switched on at $t = -\infty$.

Equation (15) can be used to calculate to first order the thermal averages

$$\langle A^\dagger_n A_m\rangle \equiv \mathrm{Tr}[\rho(t) A^\dagger_n A_m] = \mathrm{Tr}[\rho_0 A^\dagger_n(t) A_m(t)] \equiv \langle A^\dagger_n(t) A_m(t)\rangle_0, \tag{18}$$

where ρ_0 is the unperturbed density operator. One obtains

$$\langle A^\dagger_n A_m\rangle \simeq \langle A^\dagger_n A_m\rangle_0 + \Delta^{(+)}_{nm} e^{i\omega t} + \Delta^{(-)}_{nm} e^{-i\omega t}, \tag{19}$$

where the $\Delta^{(\pm)}_{nm}$ are determined by

$$\Delta^{(\pm)}_{nm} = \sum_{rs} (Q^{-1}_{nr})^* Q^{-1}_{ms}\left(\frac{\tilde{K}^{(\pm)}_{sr}\langle B^\dagger_r B_r\rangle_0}{\mp\omega + E_r - E_s + i\eta} - \frac{(\tilde{K}^{(\mp)}_{rs})^*\langle B^\dagger_s B_s\rangle_0}{\mp\omega + E_r - E_s + i\eta}\right). \tag{20}$$

Here we have made the approximation

$$\langle B^\dagger_n B_m\rangle_0 \simeq \delta_{nm}\langle B^\dagger_n B_n\rangle_0. \tag{21}$$

The neglect of the off-diagonal terms of $\langle B^\dagger_n B_m\rangle_0$ is required in order to have the thermal averages $\langle A^\dagger_n A_m\rangle$ vary periodically as given by Eq. (19). We shall see that the ansatz of Eq. (13) is dependent on having $\langle A^\dagger_n A_m\rangle$ of this form. It should be noticed that Eq. (21) would be exactly satisfied if the B_n were exact excitation operators. However, since the B_n only approximate excitation operators, the off-diagonal elements will not, in general, be zero. Green's-function methods are used in Appendix A

to evaluate $\langle B_n^\dagger B_m\rangle_0$.

The matrices $\tilde{K}^{(+)}$ and $\tilde{K}^{(-)}$ are functions of the elements of $\Delta^{(\pm)}$. In order to be specific we must give some prescription for determining K^1. We shall adopt the procedure due to Roth[8] where the matrix K in

$$[A_n, H] \simeq \sum_m K_{nm} A_m \tag{22}$$

is taken as the solution of

$$E = KN , \tag{23}$$

where the energy and normalization matrices are defined as

$$E_{nm} = \langle [[A_n, H], A_m^\dagger]_+ \rangle , \tag{24}$$

$$N_{nm} = \langle [A_n, A_m^\dagger]_+ \rangle . \tag{25}$$

Therefore, in the Roth prescription

$$K^1 = E^1 (N^0)^{-1} - K^0 N^1 (N^0)^{-1} . \tag{26}$$

Here E^1 and N^1 are the first-order differences between the perturbed and unperturbed energy and normalization matrices, respectively.

In examining whether Eq. (26) is consistent with the ansatz of Eq. (13), one encounters a difficulty due to the fact that E might contain averages of the form $\langle F_n^\dagger A_m\rangle$ where F_n is not a linear combination of the basis operators chosen. However, we shall assume that such averages can be approximated in some systematic manner in terms of averages belonging to the basis set. In that case the most general form for K^1 is clearly as given in Eq. (13) with

$$K_{nm}^{(\pm)} = M_{nm}^{(\pm)} + \sum_{rs} [\alpha_{nm}^{rs} \Delta_{rs}^{(\pm)} + \beta_{nm}^{rs} (\Delta_{rs}^{(\mp)})^*] . \tag{27}$$

Expression (27) illustrates the explicit dependence on the elements of $\Delta^{(\pm)}$ and also defines the coefficients M, α, and β. Substituting Eq. (27) into Eq. (20), one obtains an explicit equation for $\Delta^{(\pm)}$.

III. GENERALIZED SUSCEPTIBILITY IN STRONGLY CORRELATED LIMIT

The general formalism of the previous section will now be applied to the Hubbard model in order to determine the susceptibility for the paramagnetic phase in the strongly correlated limit. The treatment of electron correlation is Roth's treatment in her two-pole approximation.[6] One chooses the following set of basis operators for this application of the Roth procedure[8]:

$$\begin{aligned} A_{1k\sigma} &= c_{k\sigma} = N^{-1/2} \textstyle\sum_i c_{i\sigma} e^{i\vec{k}\cdot\vec{R}_i} , \\ A_{2k\sigma} &= d_{k\sigma} = N^{-1/2} \textstyle\sum_i n_{i-\sigma} c_{i\sigma} e^{i\vec{k}\cdot\vec{R}_i} . \end{aligned} \tag{28}$$

The unperturbed matrices E^0, N^0, and K^0 are diagonal in k and σ. One finds for E^0, N^0, and K^0 the following 2×2 matrices for each k and σ:

$$E_k^0 = \begin{pmatrix} \epsilon_k + In & (\epsilon_k + I)n \\ (\epsilon_k + I)n & In + \epsilon_k n^2 + n(1-n) W_k \end{pmatrix} , \tag{29}$$

$$N_k^0 = \begin{pmatrix} 1 & n \\ n & n \end{pmatrix} , \tag{30}$$

$$K_k^0 = \begin{pmatrix} \epsilon_k & I \\ (\epsilon_k - W_k)n & I + W_k \end{pmatrix} . \tag{31}$$

Here

$$n = \langle n_{i\sigma}\rangle_0 , \tag{32}$$

since we assume a paramagnetic phase. Also,

$$\begin{aligned} n(1-n)\, W_k \equiv & - N^{-1} \sum_{ij} T_{ij} \langle c_{i-\sigma}^\dagger c_{j-\sigma} (1 - n_{i\sigma} - n_{j\sigma})\rangle_0 \\ & + N^{-1} \sum_{ij} T_{ij} e^{i\vec{k}\cdot(\vec{R}_i - \vec{R}_j)} \\ & \times (\langle n_{i-\sigma} n_{j-\sigma}\rangle_0 - n^2 + \langle c_{i-\sigma}^\dagger c_{i\sigma} c_{j\sigma}^\dagger c_{j-\sigma}\rangle_0 \\ & - \langle c_{j-\sigma}^\dagger c_{j\sigma}^\dagger c_{i\sigma} c_{i-\sigma}\rangle_0) . \end{aligned} \tag{33}$$

The zero in energy has been chosen such that $T_{00} = 0$. The reader is referred to Roth[6] for details and for the evaluation of the zero-order averages.

The approximate excitation energies, $E_{k,\mu}$ ($\mu = 1, 2$), are found from Eq. (31) to be

$$\begin{aligned} E_{k,\mu} = \tfrac{1}{2} \{ & (\epsilon_k + I + W_k) \mp [(\epsilon_k + I + W_k)^2 \\ & - 4\epsilon_k I(1-n) - 4W_k(\epsilon_k + In)]^{1/2} \} , \end{aligned} \tag{34}$$

where the upper and lower signs refer to $\mu = 1$ and 2, respectively. The matrix Q defined by Eq. (14) is in a convenient normalization given by

$$Q_k = \begin{pmatrix} (E_{k,2} - \epsilon_k)/I & -1 \\ (E_{k,1} - \epsilon_k)/I & -1 \end{pmatrix} . \tag{35}$$

In the strongly correlated limit ($I \to \infty$) the excitation energies become

$$E_{k,1}\big|_{I\to\infty} \simeq \epsilon_k (1-n) + nW_k , \tag{36}$$

$$E_{k,2}\big|_{I\to\infty} \simeq I + \epsilon_k n + (1-n) W_k , \tag{37}$$

and Q becomes

$$Q_k\big|_{I\to\infty} = \begin{pmatrix} 1 - (\epsilon_k - W_k)(1-n)/I & -1 \\ -(\epsilon_k - W_k)n/I & -1 \end{pmatrix} . \tag{38}$$

This completes the description of the unperturbed system within the two-pole approximation for the paramagnetic phase.

In order to evaluate K^1 we must determine the matrices E and N to first order in the applied field. The perturbation as expressed by Eq. (4) may be rewritten as

$$H_1 = \tfrac{1}{2} h \sum_{k\sigma} \sigma (c_{k+q,\sigma}^\dagger c_{k\sigma} e^{i\omega t} + c_{k-q,\sigma}^\dagger c_{k\sigma} e^{-i\omega t}) , \tag{39}$$

where $h = \frac{1}{2} g \mu_B h_0$. For $q \neq 0$, the E and N matrices are clearly not diagonal in $\vec{k}$. The general elements of these matrices to first order are

$$E_{1k,1k'} = (\epsilon_k + In)\delta_{kk'} + (In_{\pm q,-\sigma} + \tfrac{1}{2}\sigma h e^{\mp i\omega t})\delta_{k\pm q,k'} , \tag{40}$$

$$E_{1k,2k'} = (\epsilon_k + I)n\delta_{kk'} + [(\epsilon_k + I)n_{\pm q,-\sigma} + n\tfrac{1}{2}\sigma h e^{\mp i\omega t}]\,\delta_{k\pm q,k'} , \tag{41}$$

$$E_{2k,1k'} = (\epsilon_k + I)n\delta_{kk'} + [(\epsilon_{k\pm q} + I)n_{\pm q,-\sigma} + s_{\pm q,-\sigma} + \tfrac{1}{2}n\sigma h e^{\mp i\omega t}]\,\delta_{k\pm q,k'} , \tag{42}$$

$$E_{2k,2k'} = [In + \epsilon_k n^2 + n(1-n)W_k]\,\delta_{kk'} + [In_{\pm q,-\sigma} + (\epsilon_k + \epsilon_{k\pm q})n_{\pm q,-\sigma}n + A^{\sigma}_{k,k\pm q} + \tfrac{1}{2}n\sigma h e^{\mp i\omega t}]\,\delta_{k\pm q,k'} , \tag{43}$$

$$N_{1k,1k'} = \delta_{kk'} , \tag{44}$$

$$N_{1k,2k'} = N_{2k,1k'} = N_{2k,2k'} = n\delta_{kk'} + n_{\pm q,-\sigma}\delta_{k\pm q,k'} , \tag{45}$$

with the following definitions:

$$n_{q\sigma} = N^{-1}\textstyle\sum_k \langle c^{\dagger}_{k+q,\sigma} c_{k\sigma}\rangle = n^{*}_{-q,\sigma} , \tag{46}$$

$$s_{q\sigma} = N^{-1}\textstyle\sum_k (\epsilon_k - \epsilon_{k+q})\langle c^{\dagger}_{k+q,\sigma} c_{k\sigma}\rangle = -s^{*}_{-q,\sigma} , \tag{47}$$

$$\begin{aligned} A^{\sigma}_{k,k+q} = &- N^{-1}\sum_{ij} T_{ij} e^{-i\vec{q}\cdot\vec{R}_i} \\ &\times\langle c^{\dagger}_{j-\sigma} c_{i-\sigma}(1 - n_{i\sigma} - n_{j\sigma} e^{i\vec{q}\cdot(\vec{R}_i - \vec{R}_j)})\rangle \\ &+ N^{-1}\sum_{ij} T_{ij} e^{i\vec{k}\cdot(\vec{R}_i - \vec{R}_j)} e^{-i\vec{q}\cdot\vec{R}_j}(\langle n_{i-\sigma} n_{j-\sigma}\rangle \\ &- \langle n_{i-\sigma}\rangle\langle n_{j-\sigma}\rangle + \langle c^{\dagger}_{i-\sigma} c_{i\sigma} c^{\dagger}_{j\sigma} c_{j-\sigma}\rangle \\ &+ \langle c^{\dagger}_{j-\sigma} c^{\dagger}_{j\sigma} c_{i\sigma} c_{i-\sigma}\rangle) . \end{aligned} \tag{48}$$

The averages in Eqs. (46)–(48) are to be evaluated to first order in the perturbation. Using Eq. (26), one obtains

$$K^{1\sigma}_{1k,1k'} = \tfrac{1}{2}\sigma h e^{\mp i\omega t}\delta_{k\pm q,k'} , \tag{49}$$

$$K^{1\sigma}_{1k,2k'} = 0 , \tag{50}$$

$$K^{1\sigma}_{2k,1k'} = \left[\left(\epsilon_{k\pm q} - \frac{n}{1-n}W_k\right)n_{\pm q,-\sigma} + \frac{1}{1-n}(s_{\pm q,-\sigma} - A^{\sigma}_{k,k\pm q})\right]\delta_{k\pm q,k'} , \tag{51}$$

$$K^{1\sigma}_{2k,2k'} = \left(\frac{1}{n(1-n)}[A^{\sigma}_{k,k\pm q} - W_k(1-2n) - ns_{\pm q,-\sigma}] + \tfrac{1}{2}\sigma h e^{\mp i\omega t}\right)\delta_{k\pm q,k'} . \tag{52}$$

It should be noticed that $A^{\sigma}_{k,k\pm q}$ as defined by Eq. (48) involves averages which are not of the form $\langle A^{\dagger}_n A_m\rangle$ where $\{A_n\}$ is the set of basis operators. Hence, Eq. (20) of the equation-of-motion method does not determine $\langle A^{\dagger}_n A_m\rangle$. In order to use Eq. (20) one must express the averages in Eq. (48) in terms of the basis set of averages. Unfortunately, there does not appear to be a unique way of doing this. For simplicity, we shall consider only the strongly correlated limit ($I \to \infty$); furthermore, we shall neglect the $\vec{k}$-dependent terms in $A^{\sigma}_{k,k\pm q}$. Neglecting the $\vec{k}$-dependent terms in $A^{\sigma}_{k,k\pm q}$ is a similar approximation to neglecting the $\vec{k}$-dependent terms in W_k. In the unperturbed system the $\vec{k}$-independent term in W_k is responsible for the desired shift in the center of gravity of the band, which makes the ferromagnetic state more likely to stabilize. The $\vec{k}$-dependent terms are small by comparison and primarily produce band narrowing. In this approximation $A^{\sigma}_{k,k\pm q}$ becomes

$$A^{\sigma}_{k,k\pm q}\big|_{I\to\infty,\, n<1/2}(\vec{k}\text{ independent}) \equiv A^{\sigma}_0 = -N^{-1}\sum_{k'} \epsilon_{k'\pm q}\langle c^{\dagger}_{k'\pm q,-\sigma} c_{k'-\sigma}\rangle . \tag{53}$$

Note that we have used the fact that in the strongly correlated limit the terms which involve a double occupancy of a given Wannier state vanish, provided $n < \frac{1}{2}$. An analogous result for $n > \frac{1}{2}$ can be obtained by making use of the electron-hole symmetry of the problem.

By neglecting the $\vec{k}$-dependent terms in $A^{\sigma}_{k,k\pm q}$ we have the desired situation where all the averages are determined by Eq. (20). Furthermore, Eq. (20) is significantly simplified by considering the strongly correlated limit. With $n < \frac{1}{2}$, only the band of energies corresponding to $E_{k,1}$ is occupied. Using Eq. (20) in the strongly correlated limit with $n < \frac{1}{2}$, we obtain for $\Delta_{k\pm q,k}$, defined by

$$\langle c^{\dagger}_{k\pm q,\sigma} c_{k\sigma}\rangle = -\sigma\Delta_{k\pm q,k} e^{\mp i\omega t} , \tag{54}$$

the following equation:

$$\Delta_{k\pm q,k} = (1-n)\left(\frac{\tilde{K}^{(\mp)}_{1k,1k\pm q} f(E_{k\pm q,1}) - (\tilde{K}^{(\pm)}_{1k\pm q,1k})^{*} f(E_{k,1})}{\pm\omega + E_{k\pm q,1} - E_{k,1} + i\eta}\right) , \tag{55}$$

where, in the approximation that $A^{\sigma}_{k,k\pm q,1k} \simeq A^{\sigma}_0$,

$$\tilde{K}^{(\mp)}_{1k,1k\pm q} = -\frac{h}{2} + \left(\epsilon_{k\pm q} - \frac{n}{1-n}W_k\right)N^{-1}\sum_{k'}\Delta_{k'\pm q,k'} + \frac{1}{1-n}N^{-1}\sum_{k'}\epsilon_{k'}\Delta_{k'\pm q,k'} , \tag{56}$$

$$(\tilde{K}^{(\pm)}_{1k\pm q,1k})^{*} = -\frac{h}{2} + \left(\epsilon_k - \frac{n}{1-n}W_{k\pm q}\right)N^{-1}\sum_{k'}\Delta_{k'\pm q,k'} + \frac{1}{1-n}N^{-1}\sum_{k'}\epsilon_{k'\pm q}\Delta_{k'\pm q,k'} . \tag{57}$$

The reduced spin susceptibility $\chi(q, \omega)$ as defined by Eq. (5) may be rewritten in terms of the $\Delta_{k\pm q,k}$ as

$$\chi(q, \omega) = [(g\mu_B)^2/h] N^{-1} \sum_k \Delta_{k+q,k} \; ; \tag{58}$$

Eq. (55) can be used to construct a set of simultaneous equations for $N^{-1}\sum_k \Delta_{k+q,k}$, $N^{-1}\sum_k \epsilon_k \Delta_{k+q,k}$, and $N^{-1}\sum_k \epsilon_{k+q} \Delta_{k+q,k}$ which can be solved for $N^{-1}\sum_k \Delta_{k+q,k}$ and thereby obtain the susceptibility. However, this set may be reduced by making use of the sum rule

$$\sum_k (\omega + \epsilon_{k+q} - \epsilon_k) \Delta_{k+q,k} = 0 \; , \tag{59}$$

which is derived in Appendix B. One finds

$$\chi(q, \omega) = \tfrac{1}{2}(g\mu_B)^2 \left(\frac{(1-n)\Gamma_0(q, \omega)}{[1+(1-n)D_0(q, \omega)][1+\Gamma_1(q, \omega)] - (1-n) D_1(q, \omega)\Gamma_0(q, \omega)} \right) \; , \tag{60}$$

where

$$\Gamma_0(q, \omega) = N^{-1} \sum_k \frac{f(E_{k,1}) - f(E_{k+q,1})}{\omega + E_{k+q,1} - E_{k,1} + i\eta} \; , \tag{61}$$

$$\Gamma_1(q, \omega) = N^{-1} \sum_k \epsilon_k \frac{f(E_{k,1}) - f(E_{k+q,1})}{\omega + E_{k+q,1} - E_{k,1} + i\eta} \; , \tag{62}$$

$$D_0(q, \omega) = -N^{-1} \sum_k \frac{[\epsilon_{k+q} - (n/(1-n)) W_k] f(E_{k+q,1}) - [\epsilon_k - (n/(1-n)) W_{k+q} - (\omega/(1-n))] f(E_{k,1})}{\omega + E_{k+q,1} - E_{k,1} + i\eta} \; , \tag{63}$$

$$D_1(q, \omega) = -N^{-1} \sum_k \epsilon_k \frac{[\epsilon_{k+q} - (n/(1-n)) W_k] f(E_{k+q,1}) - [\epsilon_k - (n/(1-n)) W_{k+q} - (\omega/(1-n))] f(E_{k,1})}{\omega + E_{k+q,1} - E_{k,1} + i\eta} \; , \tag{64}$$

and where $E_{k,1}$ is given by Eq. (36). It should be noted that Eq. (60) is an expression for the susceptibility of the paramagnetic phase in the strongly correlated limit with $n < \frac{1}{2}$. The generalization of the derivation to finite I is straightforward, provided one again neglects the $\vec{k}$-dependent part of $A^{\sigma}_{k,k+q}$. We shall not give the very complicated expression that one obtains for finite I in our approximation.

IV. DISCUSSION

Our result for $\chi(q, \omega)$ given in Eq. (60) is not the result of a strict application of a strict application of the Roth two-pole approximation to this model Hamiltonian in the strongly correlated limit. We have made the approximation of Eq. (53) which neglects the $\vec{k}$-dependent terms of $A^{\sigma}_{k,k+q}$. However, as previously discussed, we do not expect this approximation to have a significant qualitative or quantitative effect on our results. Nevertheless, we shall indicate how the $\vec{k}$-dependent terms can be included in a manner consistent with the two-pole approximation. The inclusion of these terms produces a significant complication.

For $\omega \neq 0$, it is reasonable to evaluate those averages in Eq. (48), which do not belong to the basis set, by direct substitution of Eq. (15), which gives the operators in the Heisenberg representation. The matrices $\tilde{K}^{(\mp)}$ will then depend on these averages. Consequently, they must be determined by a generalization of Eq. (20). For $\omega = 0$, it is more convenient to make use of the fact that the average are equilibrium averages. One can express these averages in terms of averages of the basis set by means of a method used by Roth[6] for evaluating W_k. This procedure is outlined in Appendix C. In the strongly correlated limit one finds

$$A^{\sigma}_{k,k+q}\big|_{I\to\infty, n<1/2, \omega=0} = n_{q,-\sigma} \sum_j T_{0j} \frac{n_j^2}{(1-2n)(1-n)} [(2-n) e^{i(\vec{k}+\vec{q})\cdot\vec{R}_j} - e^{i\vec{k}\cdot\vec{R}_j}] - N^{-1} \sum_{k'} \langle c^{\dagger}_{k'+q,-\sigma} c_{k',-\sigma} \rangle [\epsilon_{k'+q} + B_{k'}(k, k+q)] \; , \tag{65}$$

where

$$B_{k'}(k, k+q) = \sum_j T_{0j} \frac{n_j}{1-2n} [(2-n) e^{i(\vec{k}+\vec{q}+\vec{k}')\cdot\vec{R}_j} - n e^{i(\vec{k}-\vec{k}')\cdot\vec{R}_j}] \; . \tag{66}$$

This yields the situation where $\sum_{k'} \Delta_{k'+q;k'}$ is determined by an infinite set of simultaneous equations for

$$\sum_{k'} \Delta_{k'+q,k'} , \quad \sum_{k'} \epsilon_{k'} \Delta_{k'+q,k'} ,$$

and

$$\sum_{k'} B_{k'}(k, k+q)\, \Delta_{k'+q,k'}$$

for each $\vec{k}$.

However, as noted by Roth,[6] her method for evaluating W_k suffers from not being unique. One might argue that any result that depends essentially on the $\vec{k}$-dependent term of $A^{\sigma}_{k,k+q}$ are unreliable. Our approximation in this sense is of comparable validity as a strict application of the Roth two-pole approximation. The expression for $\chi(q, \omega)$ of Eq. (60) should be a valid approximation for the strongly correlated limit at higher carrier densities than can be described by the Kanamori treatment.[3] Our expression should provide the basis for a future numerical investigation of the effects of strong correlations on the frequency and wave-number dependence of the response function. In the limit $\omega \to 0$, $\chi(q, \omega)$ can be used to study instabilities toward magnetic ordering. The vanishing of $\chi^{-1}(q, 0)$ indicates the instability of the paramagnetic state against antiferromagnetic ordering of wave vector q.

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APPENDIX A

The averages $\langle B_n^{\dagger} B_m \rangle_0$ are easily evaluated within the Roth procedure by standard Green's-function techniques. One needs the Green's functions $\langle\langle A_r, A_s^{\dagger} \rangle\rangle_E^0$, where the zero superscript denotes the unperturbed Green's functions and where the notation is that of Zubarev.[9] Now in the Roth prescription[8]

$$\langle\langle A_r; A_s^{\dagger} \rangle\rangle_E^0 = \sum_p (E - K^0)^{-1}_{rp} N^0_{ps} . \tag{A1}$$

The thermal averages $\langle A_s^{\dagger} A_r \rangle_0$ are obtained from the relation

$$\langle A_s^{\dagger} A_r \rangle_0 = \mathfrak{F}_E \{ \langle\langle A_r; A_s^{\dagger} \rangle\rangle_E^0 \}$$

$$\equiv i \lim_{\eta \to 0^+} \int_{-\infty}^{+\infty} dE f(E) [\langle\langle A_r; A_s^{\dagger} \rangle\rangle^0_{E+i\eta} - \langle\langle A_r; A_s^{\dagger} \rangle\rangle^0_{E-i\eta}] , \tag{A2}$$

where $f(E)$ is the Fermi function. Therefore

$$\langle B_n^{\dagger} B_m \rangle_0 = \sum_{rs} Q^*_{ns} Q_{mr} \mathfrak{F}_E \left[\sum_p (E - K^0)^{-1}_{rp} N^0_{ps} \right] \tag{A3}$$

$$= \mathfrak{F}_E [(\omega - E_m)^{-1} (Q N^0 Q^{\dagger})_{mn}] \tag{A4}$$

$$= f(E_m) \vec{N}^0_{mn} , \tag{A5}$$

where

$$\vec{N} \equiv Q N Q^{\dagger} . \tag{A6}$$

APPENDIX B

The sum rule expressed in Eq. (59) is easily derived by considering the equation of motion of the average

$$\langle c^{\dagger}_{k \pm q, \sigma} c_{k\sigma} \rangle \equiv \mathrm{Tr} [\rho(t) c^{\dagger}_{k \pm q, \sigma} c_{k\sigma}]$$

$$= \mathrm{Tr} [\rho_0 c^{\dagger}_{k \pm q, \sigma}(t) c_{k\sigma}(t)] , \tag{B1}$$

where $\rho(t)$ and ρ_0 are the perturbed and unperturbed density operators, respectively. The perturbation is assumed to be adiabatically switched on at $t = -\infty$. The equation of motion is then

$$i \frac{d}{dt} \langle c^{\dagger}_{k \pm q, \sigma} c_{k\sigma} \rangle = \langle c^{\dagger}_{k \pm q, \sigma} [c_{k\sigma}, H] - [H, c^{\dagger}_{k \pm q, \sigma}] c_{k\sigma} \rangle . \tag{B2}$$

For $H = H_0 + H_1$, where H_0 and H_1 are given by Eqs. (1) and (4), respectively, it is straightforward to show that summing Eq. (B2) over k yields

$$i \frac{d}{dt} \sum_k \langle c^{\dagger}_{k \pm q, \sigma} c_{k\sigma} \rangle = \sum_k (\epsilon_k - \epsilon_{k \pm q}) \langle c^{\dagger}_{k \pm q, \sigma} c_{k\sigma} \rangle . \tag{B3}$$

But to first order in the perturbation $\langle c^{\dagger}_{k \pm q, \sigma} c_{k\sigma} \rangle$ is of the form given in Eq. (54). Therefore,

$$\pm \omega \sum_k \Delta_{k \pm q, k} = \sum_k (\epsilon_k - \epsilon_{k \pm q}) \Delta_{k \pm q, k} . \tag{B4}$$

APPENDIX C

We consider here the case where $\omega = 0$, and therefore the averages are equilibrium averages. In the strongly correlated limit ($I \to \infty$), the terms in Eq. (48), which involve a double occupancy of a given Wannier state, vanish. The remaining terms may be rewritten as

$$A^{\sigma}_{k,k+q} \big|_{I \to \infty} = -N^{-1} \sum_{k'} \epsilon_{k'+q} \langle c^{\dagger}_{k'+q, -\sigma} c_{k', -\sigma} \rangle$$

$$+ \sum_j T_{0j} e^{i\vec{k} \cdot \vec{R}_j} N^{-1} \sum_{k'} \Big\langle N^{-1/2} \sum_i e^{-i(\vec{k}' + \vec{q}) \cdot \vec{R}_i}$$

$$\times (n_{i+j, -\sigma} c^{\dagger}_{i, -\sigma} - \langle n_{i+j, -\sigma} \rangle\, c^{\dagger}_{i, -\sigma}$$

$$+ c^{\dagger}_{i+j, -\sigma} c_{i+j, \sigma} c^{\dagger}_{i\sigma}) c_{k', -\sigma} \Big\rangle . \tag{C1}$$

Following Roth,[6] we define operators

$$B^{1j}_{k'+q,-\sigma} \equiv N^{-1/2} \sum_i e^{-i(\vec{k}'+\vec{q})\cdot\vec{R}_i} n_{i+j,-\sigma} c^\dagger_{i-\sigma} , \quad \text{(C2)}$$

$$B^{2j}_{k'+q,\sigma} \equiv N^{-1/2} \sum_i e^{-i(\vec{k}'+\vec{q}-\vec{G}_\nu)\cdot\vec{R}_i} n_{i+j,-\sigma} c^\dagger_{i\sigma} , \quad \text{(C3)}$$

$$B^{3j}_{k'+q,-\sigma} \equiv N^{-1/2} \sum_i e^{-i(\vec{k}'+\vec{q})\cdot\vec{R}_i} c^\dagger_{i+j,-\sigma} c_{i+j,\sigma} c^\dagger_{i\sigma} . \quad \text{(C4)}$$

The equilibrium averages $\sum_{k'} \langle B^{sj}_{k'+q,\sigma} c_{k'\sigma} \rangle$ are determined by

$$\sum_{k'} \langle B^{sj}_{k'+q,\sigma} c_{k'\sigma} \rangle = \mathcal{F}_\omega \Big\{ \sum_{k'\,k} [(\omega - K)^{-1}_{1k',1k,\sigma} \langle [c_{k\sigma}, B^{sj}_{k'+q,\sigma}]_+ \rangle + (\omega - K)^{-1}_{1k',2k,\sigma} \langle [d_{k\sigma}, B^{sj}_{k'+q,\sigma}]_+ \rangle] \Big\} , \quad \text{(C5)}$$

where the only terms in the sum over k which are not zero are the k equal to k' and $k'+q$ terms. The quantities $\mathcal{F}_\omega[(\omega - K)^{-1}_{\alpha k',\beta k'+q,\sigma}]$ are easily expressed in terms of the set of thermal averages $\langle c_{k+q,\sigma} c_{k\sigma} \rangle$ and $\langle d^\dagger_{k+q,\sigma} c_{k\sigma} \rangle$, where the latter are zero in the strongly correlated limit. Therefore, Eq. (C5) yields expressions for $\sum_k \langle B^{sj}_{k'+q,\sigma} c_{k'\sigma} \rangle$ to first order in the applied field which depend on certain zero-order averages that have been evaluated by Roth[6] and averages belonging to our basis set of thermal averages. The results are substituted into Eq. (C1) in order to produce Eq. (65) for $A^\sigma_{k,k+q}$ in the strongly correlated limit when $\omega = 0$.

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†Present address: Ft. Buckner, Okinawa, APO San Francisco, Calif. 96248.

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