Electron Correlation in Ferromagnetism. III. Dynamical Susceptibility in Narrow Energy Bands

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We present our study of the dynamical susceptibility for a system of electrons in a narrow energy band. The Hamiltonian of the system consists of single-particle energies of electrons in the absence of interactions, the intra-atomic Coulomb interaction, and interatomic Coulomb and exchange interactions. An approximate expression for the susceptibility is derived by using the random-phase approximation. Instability of the paramagnetic state against the ferro- and the antiferromagnetic states is discussed. Also presented is the study of the dynamical susceptibility for a system of electrons with strong intra-atomic interactions where the validity of the random-phase approximation is dubious. In this case, in addition to the conditions for the paramagnetic instability against the ferro- and the antiferromagnetic states, we have also discussed the spin-wave excitations.

I. INTRODUCTION

The dynamical susceptibility $\chi(\vec{q}, \omega)$ of a metal is a quantity of considerable interest because it can be used to discuss a variety of problems[1]: It determines the cross section for inelastic scattering of neutrons; its poles give the frequencies of the spin waves; and the condition $\chi^{-1}(\vec{q}, 0) = 0$ gives the criterion for the stability of magnetic phases. The properties of $\chi(\vec{q}, \omega)$ for magnetic materials have so far been discussed only in terms of the most elementary models: The Heisenberg localized spin system has been discussed by Marshall,[2] by Elliott,[3] and by de Gennes[4]; the itinerant-electron model based on the Hubbard Hamiltonian[5] has been discussed within the random-phase approximation (RPA) by Izuyama *et al.*[6] and by Doniach.[7] The validity of RPA is suspect in the strongly correlated systems. Recently Sakurai[8] and Hubbard and Jain[9] have gone beyond the RPA to treat the strongly correlated systems.

The Hubbard Hamiltonian takes into account only the intra-atomic interaction. The effect of inclusion of interatomic interactions on the Hubbard Hamiltonian has been discussed by many authors.[10–12] Englert and Antonoff[13] have considered the full many-body Hamiltonian in a Bloch representation and have obtained $\chi(\vec{q}, \omega)$ within the RPA. We thought it worthwhile to investigate the dynamical susceptibility for a Hamiltonian which takes into account both intra- as well as interatomic interactions.

In this paper, we obtain the dynamical susceptibility for a model Hamiltonian which includes intra-atomic Coulomb interaction as well as interatomic Coulomb and exchange interactions between electrons in a narrow energy band. The stability conditions of magnetic states and the spin-wave dispersion relations are derived. We restrict our analysis to cases where number of electrons per atom $n_0 < 1$, since the cases $n_0 > 1$ could equivalently be treated in terms of holes in the band.

In Sec. II we write the Hamiltonian of the system in the Wannier representation and give a brief survey of the Green's-function technique. In Sec. III, we obtain the dynamical susceptibility using the random-phase approximation. Instability of paramagnetic state against ferro- and antiferromagnetic states is discussed. In Sec. IV, we derive an expression for the dynamical susceptibility for strongly correlated systems and discuss the stability of magnetic states and the spin-wave dispersion relations. In Sec. V, we summarize our conclusions.

II. HAMILTONIAN AND GREEN'S FUNCTION

We consider a system of electrons in a band which interact with one another via the Coulomb interaction. The one-band Hamiltonian for the system in the Wannier representation can be written in the second-quantized form,

$$H = \sum_{ij\sigma} \epsilon_{ij} a^{\dagger}_{i\sigma} a_{j\sigma} + \tfrac{1}{2} \sum_{ijkl;\sigma\sigma'} V_{ijkl} a^{\dagger}_{i\sigma} a^{\dagger}_{j\sigma'} a_{k\sigma'} a_{l\sigma} \quad , \qquad (1)$$

where

$$\epsilon_{ij} = \int \phi^{*}_{i}(\vec{r}) \left[-\nabla^2/2m + V_c(\vec{r}) \right] \phi_j(\vec{r}) \, d^3r \, ,$$

$$V_{ijkl} = \int\int \phi^{*}_{i}(\vec{r}) \phi^{*}_{j}(r') \frac{e^2}{|\vec{r} - \vec{r}'|} \phi_k(\vec{r}') \phi_l(\vec{r}) \, d^3r \, d^3r' \, ,$$

where $a^{\dagger}_{i\sigma}$, $a_{i\sigma}$ are the creation and annihilation operators for an electron of spin σ at the lattice site i. $\phi_i(\vec{r})$ is the Wannier wave function at the lattice site i, $V_c(\vec{r})$ is the periodic potential due to ions, and $-\nabla^2/2m$ is the kinetic energy of the electron. Here and hereafter we use the units where $\hbar = 1$. V_{ijkl} are, in general, four-center integrals which are extremely difficult to compute. For narrow energy bands three- and four-center integrals are very small in comparison to two- and one-center

integrals. Therefore, we simplify (1) by retaining only one- and two-center integrals. Of all the two-center integrals we keep only two of them namely, the interatomic Coulomb interaction V_{iji} and the interatomic exchange interaction $V_{ij\,ij}$. Then the Hamiltonian (1) can be represented in the form

$$H=\sum_{ij\sigma}\epsilon_{ij}\,a^{\dagger}_{i\sigma}a_{j\sigma}+(I/2)\sum_{i\sigma}n_{i\sigma}n_{i\,-\sigma}$$
$$+\tfrac{1}{2}\sum_{ij;\sigma\sigma'}V_{ij}n_{i\sigma}n_{j\sigma'}+\tfrac{1}{2}\sum_{ij;\sigma\sigma'}J_{ij}a^{\dagger}_{i\sigma}a^{\dagger}_{j\sigma'}a_{i\sigma'}a_{j\sigma}\ , \quad (2)$$

where

$$I=V_{iiii},\quad V_{ij}=V_{ijji},\quad J_{ij}=V_{ij\,ij},\quad n_{i\sigma}=a^{\dagger}_{i\sigma}a_{i\sigma}\ .$$

Here we have assumed that $V_{ii}=J_{ii}=0$. Throughout this treatment we shall restrict ourselves to nearest-neighbor interatomic interactions, which is reasonable in narrow energy bands. The parameters I, V, J, and ϵ should be taken as phenomenological quantities. In relating their values to properties of real solids, one should realize that these parameters contain contributions due to indirect interactions involving other bands; for example, the interaction between "magnetic" electrons in a metal is screened by conduction electrons in a higher conduction band.

The dynamical susceptibility of the system can be expressed in terms of double-time retarded Green's function.[6] A conventional definition of retarded Green's function is[14]

$$\langle\langle A(t);\,B\rangle\rangle=-i\theta(t)\langle[A(t),B]_{\eta}\rangle\ , \quad (3)$$

where $\theta(t)$ is the Heaviside unit step function, the angular brackets $\langle\ \rangle$ denote a grand canonical ensemble average, namely,

$$\langle O\rangle=\mathrm{Tr}e^{-\beta(H-\mu Ne)}O/\mathrm{Tr}e^{-\beta(H-\mu Ne)}\ ,$$

where μ is the chemical potential, Ne is the total electron number operator, $\beta=1/k_BT$, k_B is the Boltzmann constant, and T is the absolute temperature.

We have

$$A(t)=e^{iHt}Ae^{-iHt}\ ,$$

and $[A,\,B]_{\eta}=AB+\eta BA$, $\eta=\pm1$ (whichever is more convenient). The Green's function (3) satisfies the equation of motion[14]

$$\omega\langle\langle A;B\rangle\rangle_{\omega}=\frac{1}{2\pi}\langle[A,\,B]_{\eta}\rangle+\langle\langle[A,\,H]_{-};B\rangle\rangle_{\omega}\ , \quad (4)$$

where the Fourier transform $\langle\langle A;B\rangle\rangle_{\omega}$ is defined by

$$\langle\langle A;B\rangle\rangle_{\omega}=\frac{1}{2\pi}\int_{-\infty}^{\infty}\langle\langle A(t);B\rangle\rangle\,e^{i\omega t}\,dt\ . \quad (5)$$

The dynamical susceptibility $\chi_{-+}(\vec{q},\,\omega)$ corresponding to a process with spin flip is given by[6]

$$\chi_{-+}(\vec{q},\,\omega)=-2\pi(g\mu_BN)^2\langle\langle n^{-+}(\vec{q});n^{+-}(-\vec{q})\rangle\rangle_{-\omega}\qquad(\eta=-1)\ , \quad (6)$$

where g is the Lande's splitting factor, μ_B is the Bohr magneton, N is the number of atoms, and spin-density operator $n^{\sigma\sigma'}(\vec{q})$ is defined as

$$n^{\sigma\sigma'}(\vec{q})=\frac{1}{N}\sum_{\vec{k}}n^{\sigma\sigma'}_{\vec{k}}(\vec{q})\ ,\quad n^{\sigma\sigma'}_{\vec{k}}(\vec{q})=a^{\dagger}_{(\vec{k}+\vec{q})\sigma}a_{\vec{k}\sigma'}\ . \quad (7)$$

The Bloch operators $a_{k\sigma}$ and $a^{\dagger}_{k\sigma'}$ are defined by

$$a_{\vec{k}\sigma}=N^{-1/2}\textstyle\sum_i e^{-i\vec{k}\cdot\vec{R}_i}a_{i\sigma}\ ,$$
$$a^{\dagger}_{\vec{k}\sigma}=N^{-1/2}\textstyle\sum_i e^{i\vec{k}\cdot\vec{R}_i}a^{\dagger}_{i\sigma}\ . \quad (8)$$

III. WEAK-INTRA-ATOMIC-INTERACTION THEORY

For the sake of comparison with the results of the strong-intra-atomic-interaction theory developed in Sec. IV, it is desirable to investigate the results obtained by applying the random-phase approximation which is justified only when the intra-atomic interaction I is small as compared to the bandwidth $\alpha(I\ll\alpha)$.[15] To evaluate the dynamical susceptibility $\chi_{-+}(\vec{q},\,\omega)$, we follow a procedure similar to that of Izuyama *et al.*[6] for the Hubbard model. We first evaluate the retarded Green's function

$$\langle\langle n^{-+}(\vec{q});n^{+-}(-\vec{q})\rangle\rangle_{\omega}=(1/N)\textstyle\sum_{\vec{k}}\langle\langle n^{-+}_{\vec{k}}(\vec{q});n^{+-}(-\vec{q})\rangle\rangle_{\omega}\ . \quad (9)$$

This retarded Green's function may be obtained by its equation of motion. For each term of the sum on the right-hand side of (9) we have

$$\omega\langle\langle n^{-+}_{\vec{k}}(\vec{q});\,n^{+-}(-\vec{q})\rangle\rangle_{\omega}=\frac{1}{2\pi}\langle[n^{-+}_{\vec{k}}(\vec{q}),\,n^{+-}(-\vec{q})]_{-}\rangle$$
$$+\langle\langle[n^{-+}_{\vec{k}}(\vec{q}),H]_{-};n^{+-}(-\vec{q})\rangle\rangle_{\omega}\ . \quad (10)$$

For the Hamiltonian (2) the commutator $[n^{-+}_{\vec{k}}(\vec{q}),H]_{-}$ consists of many terms and a rigorous treatment is prohibitively difficult. Accordingly, we retain only those terms that can be transformed into a form like $a^{\dagger}_{k\sigma}a_{k\sigma}n^{-+}_{k}(\vec{q})$ and ignore the rest of them.[6] This approximation corresponds to the RPA. Further, the chain of successive Green's functions is cut off by the approximation

$$\langle\langle a^{\dagger}_{\vec{k}\sigma}a_{\vec{k}\sigma}n^{-+}_{\vec{k}}(\vec{q});n^{+-}(-\vec{q})\rangle\rangle_{\omega}$$
$$\simeq\langle a^{\dagger}_{\vec{k}\sigma}a_{\vec{k}\sigma}\rangle\langle\langle n^{-+}_{\vec{k}}(\vec{q});\,n^{+-}(-\vec{q})\rangle\rangle_{\omega}\ . \quad (11)$$

In this approximation the equation of motion (10) is reduced to the form

$$\omega\langle\langle n^{-+}_{\vec{k}}(\vec{q});\,n^{+-}(-\vec{q})\rangle\rangle_{\omega}=\frac{1}{2\pi}\langle[n^{-+}_{\vec{k}}(\vec{q}),\,n^{+-}(-\vec{q})]_{-}\rangle+\Big(\epsilon_{\vec{k}}-\epsilon_{\vec{k}+\vec{q}}-(I+J_0)\sum_{\sigma}\sigma\langle n^{\sigma\sigma}(0)\rangle+\frac{1}{N}\sum_{\vec{k}'\sigma}(J_{\vec{k}'-\vec{k}}-J_{\vec{k}'-\vec{k}+\vec{q}})\langle a^{\dagger}_{\vec{k}'\sigma}a_{\vec{k}'\sigma}\rangle$$

$$-\frac{1}{N}\sum_{\vec{k}'} V_{\vec{k}'-\vec{k}-\vec{q}}\langle a^{\dagger}_{\vec{k}'+}a_{\vec{k}'+}\rangle+\frac{1}{N}\sum_{\vec{k}'} V_{\vec{k}'-\vec{k}}\langle a^{\dagger}_{\vec{k}'-}a_{\vec{k}'-}\rangle\Big)\langle\langle n^{-+}_{\vec{k}}(\vec{q});\ n^{+-}(-\vec{q})\rangle\rangle_{\omega}$$

$$+\frac{1}{N}(I+J_{\vec{q}})(\langle a^{\dagger}_{\vec{k}+}a_{\vec{k}+}\rangle-\langle a^{\dagger}_{\vec{k}+\vec{q}-}a_{\vec{k}+\vec{q}-}\rangle)\sum_{\vec{k}}\langle\langle n^{-+}_{\vec{k}}(\vec{q});\ n^{+-}(-\vec{q})\rangle\rangle_{\omega}$$

$$+\frac{1}{N}\sum_{\vec{k}'} V_{\vec{k}'-\vec{k}}(\langle a^{\dagger}_{\vec{k}'+}a_{\vec{k}'+}\rangle-\langle a^{\dagger}_{\vec{k}'+\vec{q}-}a_{\vec{k}'+\vec{q}-}\rangle)\langle\langle n^{-+}_{\vec{k}'}(\vec{q});\ n^{+-}(-\vec{q})\rangle\rangle_{\omega}\ , \qquad (12)$$

where $\epsilon_{\vec{k}}$, $V_{\vec{k}}$, and $J_{\vec{k}}$ are defined by

$$\epsilon_{ij}=\frac{1}{N}\sum_{\vec{k}}\epsilon_{\vec{k}}e^{i\vec{k}\cdot(\vec{R}_i-\vec{R}_j)}\ , \qquad (13)$$

$$V_{ij}=\frac{1}{N}\sum_{\vec{k}} V_{\vec{k}}e^{i\vec{k}\cdot(\vec{R}_i-\vec{R}_j)}\ , \qquad (14)$$

$$J_{ij}=\frac{1}{N}\sum_{\vec{k}} J_{\vec{k}}\ e^{i\vec{k}\cdot(\vec{R}_i-\vec{R}_j)}\ . \qquad (15)$$

Hereafter we shall assume that $\epsilon_{ii}=(1/N)\sum_{\vec{k}}\epsilon_{\vec{k}}=0$, i.e., we measure the energy from the middle of the band $\epsilon_{\vec{k}}$. The quantities $V_{\vec{k}}$, $J_{\vec{k}}$ vary from $-V_0$, $-J_0$ to V_0, J_0 inside a Brillouin zone. Hence, one may expect the terms which contain V's and J's under the summation sign to be quite small in comparison to other terms. We neglect these terms and hope that such an approximation will not affect qualitatively the nature of the solutions, because these solutions involve a linear combination of the Green's functions $\langle\langle n^{-+}_{\vec{k}}(\vec{q});\ n^{+-}(-\vec{q})\rangle\rangle_{\omega}$ for all $\vec{k}$.[13] By incorporating this approximation in Eq. (12), we get

$$[\omega-\epsilon_{\vec{k}}+\epsilon_{\vec{k}+\vec{q}}+(I+J_0)\textstyle\sum_{\sigma}\sigma\langle n^{\sigma\sigma}(0)\rangle]\langle\langle n^{-+}_{\vec{k}}(\vec{q});\ n^{+-}(-\vec{q})\rangle\rangle_{\omega}$$
$$=(1/2\pi)\langle[n^{-+}_{\vec{k}}(\vec{q}),\ n^{+-}(-\vec{q})]_-\rangle$$
$$+(I+J_{\vec{q}})(\langle a^{\dagger}_{\vec{k}+}a_{\vec{k}+}\rangle-\langle a^{\dagger}_{\vec{k}+\vec{q}-}a_{\vec{k}+\vec{q}-}\rangle)$$
$$\times\langle\langle n^{-+}(\vec{q});\ n^{+-}(-\vec{q})\rangle\rangle_{\omega}\ .$$

Dividing both sides of this equation by

$$\omega-\epsilon_{\vec{k}}+\epsilon_{\vec{k}+\vec{q}}+(I+J_0)\textstyle\sum_{\sigma}\sigma\langle n^{\sigma\sigma}(0)\rangle\ ,$$

and summing up over all wave vectors $\vec{k}$ we obtain the Green's function $\langle\langle n^{-+}(\vec{q});\ n^{+-}(-\vec{q})\rangle\rangle_{\omega}$ and hence the dynamical susceptibility

$$\chi_{-+}(\vec{q},\omega)=\frac{-g^2\mu_B^2\ \Gamma_{-+}(\vec{q},\omega)}{1+[(I+J_{\vec{q}})/N]\,\Gamma_{-+}(\vec{q},\omega)}\ , \qquad (16)$$

where

$$\Gamma_{-+}(\vec{q},\omega)=\textstyle\sum_{\vec{k}}\dfrac{\langle a^{\dagger}_{\vec{k}+\vec{q}-}a_{\vec{k}+\vec{q}-}\rangle-\langle a^{\dagger}_{\vec{k}+}a_{\vec{k}+}\rangle}{-\omega-\epsilon_{\vec{k}}+\epsilon_{\vec{k}+\vec{q}}+(I+J_0)\sum_{\sigma}\sigma\langle n^{\sigma\sigma}(0)\rangle}\ . \qquad (17)$$

An expression for the dynamical susceptibility similar to that of (16) has also been obtained by Englert and Antonoff.[13] In the absence of interatomic interactions, Eq. (16) reduces to that obtained by Izuyama *et al.*[6] The averages $\langle a^{\dagger}_{\vec{k}\sigma}a_{\vec{k}\sigma}\rangle$ appearing in Eq. (17) can be obtained from the knowledge of the one-particle Green's function $\langle\langle a_{\vec{k}\sigma};\ a^{\dagger}_{\vec{k}\sigma}\rangle\rangle_{\omega}$ $(\eta=-1)$. In the Appendix we have shown that

$$\langle a^{\dagger}_{\vec{k}\sigma}a_{\vec{k}\sigma}\rangle=f(\epsilon_{\vec{k}}+I\langle n^{-\sigma-\sigma}(0)\rangle+V_0n_0-J_0\langle n^{\sigma\sigma}(0)\rangle)\ . \qquad (18)$$

Here, $n_0=\sum_{\sigma}\langle n^{\sigma\sigma}(0)\rangle$ denotes the number of electrons per atom and $f(\omega)=(e^{\beta(\omega-\mu)}+1)^{-1}$ is the Fermi distribution function.

The denominator of the susceptibility (16) gives the dispersion relations of spin waves and the conditions for the stability of magnetic phases. Spin-wave excitations have been discussed by Englert and Antonoff[13] and Izuyama *et al.*[6] Recently, Penn[16] has discussed the stability of magnetic phase for the Hubbard model in the self-consistent field approximation. Here, we shall discuss the effect of interatomic interactions on the instability of the paramagnetic state against the ferro- and the antiferromagnetic states. The paramagnetic state is unstable against the ferro- and antiferromagnetic states when, respectively, the susceptibilities $\chi(0,0)=\chi_{-+}(0,0)$ and $\chi(\vec{Q},0)=\chi_{-+}(\vec{Q},0)$ in the paramagnetic state diverge. Here, $\vec{Q}$ is half of the smallest reciprocal-lattice vector. From Eqs. (16)–(18), the susceptibilities $\chi(0,0)$ and $\chi(\vec{Q},0)$ are given as

$$\chi(0,0)=\frac{-g^2\mu_B^2\ \Gamma(0,0)}{1+[(I+J_0)/N]\ \Gamma(0,0)}\ , \qquad (19)$$

$$\chi(\vec{Q},0)=\frac{-g^2\mu_B^2\Gamma(\vec{Q},0)}{1+[(J-J_0)/N]\Gamma(\vec{Q},0)}\ , \qquad (20)$$

where

$$\Gamma(0,0)=-\beta\textstyle\sum_{\vec{k}} f(\epsilon_{\vec{k}}+(I+2V_0-J_0)\frac{1}{2}n_0)$$
$$\times[1-f(\epsilon_{\vec{k}}+(I+2V_0-J_0)\tfrac{1}{2}n_0)] \qquad (21)$$

and

$$\Gamma(\vec{Q},0)=-\sum_{\vec{k}\sigma}\sigma\frac{f(-\sigma\epsilon_{\vec{k}}+(I+2V_0-J_0)n_0/2)}{2\epsilon_{\vec{k}}}\ . \qquad (22)$$

In deriving Eqs. (20) and (22), we have made use of the fact that $\epsilon_{\vec{k}+\vec{Q}}=-\epsilon_{\vec{k}}$ and $J_{\vec{Q}}=-J_0$, if ϵ_{ij} and J_{ij} are nonzero only when i and j are nearest-neighbor lattice sites. The chemical potential μ in the paramagnetic state is determined by

$$\frac{n_0}{2} = \frac{1}{N}\sum_{\vec{k}} f(\epsilon_{\vec{k}} + (I + 2V_0 - J_0)\tfrac{1}{2}n_0) \quad . \tag{23}$$

A. Instability of Paramagnetic State against Ferromagnetic State

1. *Zero Bandwidth*

For zero bandwidth $\epsilon_{\vec{k}} = 0$ for all $\vec{k}$, and hence Eq. (23) reduces to

$$f((I + 2V_0 - J_0)\tfrac{1}{2}n_0) = \tfrac{1}{2}n_0 \quad . \tag{24}$$

By substituting the value of the Fermi function from Eq. (24) in Eq. (21), we get

$$\Gamma(0,0) = -\tfrac{1}{4}[\beta N(2 - n_0)n_0] \quad ,$$

which on substituting in Eq. (19) gives the Curie-Weiss law

$$\chi(0,0) = C/(T - T_c) \quad , \tag{25}$$

where

$$C = Ng^2\mu_B^2(2 - n_0)n_0/4k_B$$

is the Curie-Weiss constant and

$$T_c = (I + J_0)(2 - n_0)n_0/4k_B$$

is the critical temperature at which the instability of the paramagnetic state occurs. It should be noted that both C and T_c depend on the number of electrons per atom n_0. For $n_0 = 1$ and in the absence of interatomic interactions, T_c reduces to a value obtained by Morris and Cornwell.[17] In the absence of intra-atomic interaction I, for one electron per atom, the value of T_c is given by $J\beta_c = 4/z$, where J $(J = J_0/z)$ is the nearest-neighbor exchange interaction and z is the number of nearest neighbors. For sc, bcc, and fcc lattices, the values of $J\beta_c$ are 0.66, 0.5, and 0.33, respectively. These values can be compared with the values 0.5972, 0.3963, and 0.2492 obtained by high-temperature power-series expansion of the susceptibility for the spin-$\frac{1}{2}$ Heisenberg model.[18] The values of $J\beta_c$ obtained here are just double those obtained by the molecular-field theory of the Heisenberg model.

2. *Finite Bandwidth*

At absolute zero of temperature, the Fermi distribution function $f(\epsilon)$ can be replaced by $\theta(\mu - \epsilon)$. By making use of the identity $d\theta(\epsilon)/d\epsilon \equiv \delta(\epsilon)$ in Eq. (19), the dynamical susceptibility $\chi(0,0)$ can be obtained as

$$\chi(0,0) = \frac{Ng^2\mu_B^2\,\rho(\mu - (I + 2V_0 - J_0)\tfrac{1}{2}n_0)}{1 - (I + J_0)\rho(\mu - (I + 2V_0 - J_0)\tfrac{1}{2}n_0)} \quad , \tag{26}$$

where $\rho(\omega) = (1/N)\sum_{\vec{k}} \delta(\omega - \epsilon_{\vec{k}})$ is the density of states for the band $\epsilon_{\vec{k}}$. The denominator of Eq. (26) gives the Stoner criterion[19] for the instability of the paramagnetic state

$$1 - (I + J_0)\rho(\mu - (I + 2V_0 - J_0)\tfrac{1}{2}n_0) \leq 0 \quad . \tag{27}$$

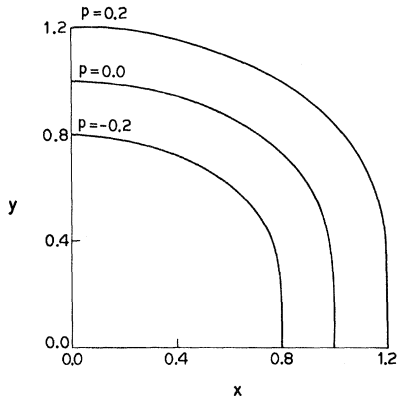

FIG. 1. Plot of the critical temperature $(y = 4k_BT_c/I)$ as a function of bandwidth $(x = \alpha/I)$ for various ratios $p = J_0/I$.

At finite temperatures, we restrict ourselves to $n_0 = 1$, because in this case Eqs. (19), (21), and (23) are considerably simplified. In fact, Eq. (23) is satisfied for $\mu = \frac{1}{2}(I + 2V_0 - J_0)$ and therefore Eq. (19) reduces to

$$\chi(0,0) = -g^2\mu_B^2 N \int \rho(\epsilon)\frac{df(\epsilon)}{d\epsilon}\,d\epsilon \Big/ \left(1 + (I + J_0)\int \rho(\epsilon)\frac{df(\epsilon)}{d\epsilon}\,d\epsilon\right) \quad . \tag{28}$$

To evaluate Eq. (28), one has to choose a particular form of the density of states $\rho(\epsilon)$. For simplicity, we choose a square density of states defined by

$$\rho(\epsilon) = 1/\alpha \quad \text{if } -\tfrac{1}{2}\alpha < \epsilon < \tfrac{1}{2}\alpha$$
$$= 0 \quad \text{otherwise} \quad . \tag{29}$$

For this density of states, Eq. (28) reduces to

$$\chi(0,0) = \frac{(g^2\mu_B^2 N/\alpha)\tanh(\frac{1}{4}\beta\alpha)}{1 - [(I + J_0)/\alpha]\tanh(\frac{1}{4}\beta\alpha)} \quad . \tag{30}$$

The denominator of the right-hand side of Eq. (30) gives the critical temperature

$$T_c = \frac{\alpha/4k_B}{\tanh^{-1}[\alpha/(I + J_0)]} \, . \tag{31}$$

In Fig. 1 we have shown the variation of $4k_BT_c/I$ as a function of α/I for various values of J_0/I.

B. Instability of Paramagnetic State against Antiferromagnetic State

1. *Zero Bandwidth*

It can readily be shown from Eqs. (22) and (24) on expanding the Fermi distribution function at $\epsilon_{\vec{k}} = 0$ by Taylor's series that for zero bandwidth,

$$\Gamma(\vec{Q}, 0) = -\tfrac{1}{4}N\beta n_0(2 - n_0) \quad ,$$

which, when substituted in Eq. (20), gives us

$$\chi(\vec{Q}, 0) = C/(T - T_N) , \tag{32}$$

where $T_N = (I - J_0)n_0(2 - n_0)/4k_B$ is the Néel temperature. For one electron per atom T_N reduces to a value obtained by Morris and Cronwell[17] in the absence of interatomic interactions. If we compare the Néel temperature T_N with the Curie temperature T_c obtained in Sec. III A 2, we see that for positive J_0, $T_c > T_N$, and for negative J_0, $T_c < T_N$. This result can only be obtained by the combined effect of intra-atomic and interatomic exchange interaction. Either of these two interactions alone cannot give such type of behavior. This behavior of the model suggests that perhaps the combined effect of intra- as well as interatomic interactions may be fruitful to explain the magnetic phase diagrams of the rare-earth elements.[20]

2. *Finite Bandwidth*

We shall discuss the finite bandwidth case separately both at absolute zero of temperature and at finite temperatures. At absolute zero of temperature, by replacing the Fermi distribution function by a θ function, the denominator of Eq. (20) gives the condition for the paramagnetic instability as

$$1 - \frac{I - J_0}{2} \int d\epsilon \, \frac{\rho(\epsilon)}{\epsilon} \times \sum_{\sigma} \sigma\theta\left(-\sigma\epsilon + \mu - (I + 2V_0 - J_0)\tfrac{1}{2}n_0\right) \leq 0 .$$

For a square density of states defined by (29), it reduces to

$$\frac{I}{\alpha} \geq \frac{J_0}{\alpha} + \frac{1}{|\ln(1 - n_0)|} . \tag{33}$$

The sign of equality in (33) gives the boundary line between para- and antiferromagnatic states. In Fig. 2 we have plotted I/α vs n_0 for various values of J_0/α. In the region above the dashed curves, antiferromagnetic states are more stable than the paramagnetic states, while in the region below the dashed curves, the paramagnetic states are more stable than the antiferromagnetic states. We have also shown by solid lines the boundary between the para- and ferromagnetic states [from (27) for square density of states the boundary line between para- and ferromagnetic states is given by $I/\alpha = 1 - J_0/\alpha$]. The region above the solid lines corresponds to the stability of ferromagnetic states against the paramagnetic state, and in the region below the solid lines the reverse holds true. For half-filled band ($n_0 = 1$), the paramagnetic state is always unstable against ferro- or antiferromagnetic states when $1 < J_0/\alpha < 0$; for $0 < J_0/\alpha < 1$ the paramagnetic state is more stable than both ferro- and antiferromagnetic states when $I/\alpha < 1 - J_0/\alpha$. Thus, the prediction of Penn[16] that for half-filled band the paramagnetic state is not possible, no longer holds good when we take interatomic interactions into account.

At finite temperatures, for the reasons given in Sec. III A 2, we restrict ourselves to the case $n_0 = 1$. From (20) the instability of the paramagnetic state against the antiferromagnetic state is given by

$$1 - \frac{I - J_0}{2N} \sum_{\vec{k}} \frac{\tanh \frac{1}{2}\beta\epsilon_{\vec{k}}}{\epsilon_{\vec{k}}} \leq 0 . \tag{34}$$

In the absence of interatomic interactions, this inequality has recently been obtained by Langer *et al.*[21] with the help of a one-particle Green's function by assuming a two-sublattice model for the antiferromagnetic system. For sc lattice they have plotted the transition temperature as a function of I ($J_0 = 0$). From this curve, it is clear that if we replace I by $(I - J_0)$, then for each value of I the transition temperature decreases for positive J_0 and increases for negative J_0.

IV. STRONG-INTRA-ATOMIC-INTERACTION THEORY

In this section we develop a theory when the intra-atomic interaction I is very large in absolute magnitude as compared to the interatomic couplings ϵ_{ij}, V_{ij}, and J_{ij}. In Hamiltonian (2), I represents the energy required to bring two electrons into the same atomic state. Consequently, for sufficiently large $I(\gg |\epsilon_{ij}|, |V_{ij}|, |J_{ij}|)$ such doubly occupied atomic states cannot occur in the low-lying states of the entire system except in virtual transitions. It is well known that such transitions lead to renormalizations of the interactions in the system. The transitions to doubly occupied atomic states, which occur only in virtual processes, may be accounted for by renormalizing the parameters ϵ_{ij}, V_{ij}, and J_{ij}. Because of the exclusion of doubly occupied states, the intra-atomic interactions serve to reduce the phase space available to the electronic system. In order to formulate this effect, we first represent the states that are available to the system as vectors in a Hilbert space S_0. Correspondingly, the observables are represented by a set of operators Q_0 on S_0. We then take account of the fact that the intra-atomic interactions exclude state vectors from a well-defined set in S_0, which means that they confine the states to a subspace S of S_0. Consequently, the observables are now represented by operators Q on S. These are related to the corresponding primitive operators Q_0 by the formula

$$Q = PQ_0P , \tag{35}$$

where P is the projection operator for S. The algebra of the set $\{Q\}$ is quite different from that of $\{Q_0\}$. This difference represents the changes in the properties of the system due to correlations introduced by intra-atomic interactions. In other words, the effect of these interactions are built into

our formalism through the new algebra of the operators on the reduced Hilbert space S.

Let $b_{\vec{k}\sigma}$, $b^{\dagger}_{\vec{k}\sigma}$, and $\nu^{\sigma\sigma'}_{(\vec{k})}$ be the operators in the subspace S corresponding to the operators $a_{\vec{k}\sigma}$, $a^{\dagger}_{\vec{k}\sigma}$, and $n^{\sigma\sigma'}_{(\vec{k})}$ in the space S_0. It can be shown that the operators $b_{\vec{k}\sigma}$, $b^{\dagger}_{\vec{k}\sigma}$, and $\nu^{\sigma\sigma'}_{(\vec{k})}$ satisfy the algebraic relations[10]

$$
\begin{aligned}
&[b_{\vec{k}\sigma}, b^{\dagger}_{\vec{k}'\sigma'}]_+ = [\delta_{\vec{k}\vec{k}'} - \nu^{-\sigma-\sigma}_{(\vec{k}'-\vec{k})}]\,\delta_{\sigma\sigma'} + \delta_{\sigma-\sigma'}\,\nu^{\sigma-\sigma}_{(\vec{k}'-\vec{k})} \quad ,\\
&[b_{\vec{k}\sigma}, b_{\vec{k}'\sigma'}]_+ = [b^{\dagger}_{\vec{k}\sigma}, b^{\dagger}_{\vec{k}'\sigma'}]_+ = 0 \quad , \qquad (36)\\
&[b_{\vec{k}\sigma}, \nu^{\sigma_1\sigma_2}_{(\vec{k}'-\vec{k})}]_- = \frac{1}{N}\, b_{(\vec{k}-\vec{k}')\sigma_2}\,\delta_{\sigma\sigma_1} \quad .
\end{aligned}
$$

In terms of the operators in the subspace S the Hamiltonian (2) can be written

$$
H = \sum_{\vec{k}\sigma} \epsilon_{\vec{k}}\, b^{\dagger}_{\vec{k}\sigma}\, b_{\vec{k}\sigma} + N\sum_{\vec{k}} K_{\vec{k}}\,\nu_{\vec{k}}\,\nu_{-\vec{k}} + N\sum_{\vec{k}} \tilde{J}_{\vec{k}}\,\vec{S}_{\vec{k}}\cdot\vec{S}_{-\vec{k}} \quad , \qquad (37)
$$

where

$$
K_{\vec{k}} = \tfrac{1}{2}\,[V(\vec{k}) - J(\vec{k})] \quad , \qquad (38)
$$

$$
\tilde{J}_{\vec{k}} = -\tfrac{1}{4}\,J(\vec{k}) \quad , \qquad (39)
$$

$$
\nu_{\vec{k}} = \textstyle\sum_{\sigma} \nu^{\sigma\sigma}_{(\vec{k})} \quad , \qquad (40)
$$

$$
\vec{S}_{\vec{k}} = \textstyle\sum_{\sigma} \{\nu^{\sigma-\sigma}_{(\vec{k})}, -i\sigma\,\nu^{\sigma-\sigma}_{(\vec{k})}\} \quad . \qquad (41)
$$

The dynamical susceptibility $\chi_{-+}(\vec{q}, \omega)$ is given by

$$
\chi_{-+}(\vec{q}, \omega) = -(g\mu_B N)^2 \langle\langle \nu^{-+}(\vec{q});\ \nu^{+-}(-\vec{q})\rangle\rangle_{-\omega} \quad . \qquad (42)
$$

To evaluate $\chi_{-+}(\vec{q}, \omega)$ we proceed in a manner similar to that adopted in Sec. III. We write the equation of motion for the Green's function

$$
\langle\langle \nu^{-+}_{k}(\vec{q});\ \nu^{+-}(-\vec{q})\rangle\rangle_{\omega} \quad , \quad [\nu^{\sigma\sigma'}_{k}(\vec{q}) = b^{\dagger}_{(\vec{k}+\vec{q})\sigma}\, b_{\vec{k}\sigma'}] \quad ,
$$

$$
\omega\,\langle\langle \nu^{-+}_{\vec{k}}(\vec{q});\ \nu^{+-}(-\vec{q})\rangle\rangle_{\omega} = \frac{1}{2\pi}\,\langle [\nu^{-+}_{\vec{k}}(\vec{q}),\ \nu^{+-}(-\vec{q})]_-\rangle
$$

$$
+ \langle\langle [\nu^{-+}_{\vec{k}}(\vec{q}),\ H]_-;\ \nu^{+-}(-\vec{q})\rangle\rangle_{\omega} \quad . \qquad (43)
$$

For the Hamiltonian (37), we have

$$
\begin{aligned}
[\nu^{-+}_{\vec{k}}(\vec{q}),\ H]_- = &-\sum_{\vec{k}_1} \epsilon_{\vec{k}_1}\,[\delta_{\vec{k}+\vec{q},\vec{k}_1} - \nu^{-\sigma-\sigma}_{(\vec{k}+\vec{q}-\vec{k}_1)}]\, b^{\dagger}_{\vec{k}_1\sigma}\, b_{\vec{k}-\sigma} - \sum_{\vec{k}_1} \epsilon_{\vec{k}_1}\,\nu^{-\sigma-\sigma}_{(\vec{k}+\vec{q}-\vec{k}_1)}\, b^{\dagger}_{\vec{k}_1-\sigma} b_{\vec{k}-\sigma} - 2\sum_{\vec{k}_1\sigma_1} K_{\vec{k}_1}\,\nu^{\sigma\sigma_1}(-\vec{k}_1)\, b^{\dagger}_{\vec{k}+\vec{q}+\vec{k}_1\sigma}\, b_{\vec{k}-\sigma}\\
&- 4\sum_{\vec{k}_1} \tilde{J}_{\vec{k}_1}\,\nu^{\sigma-\sigma}(-\vec{k}_1)\, b^{\dagger}_{\vec{k}+\vec{q}+\vec{k}_1-\sigma}\, b_{\vec{k}-\sigma} - 4\sum_{\vec{k}_1\sigma} \tilde{J}_{\vec{k}_1}\,\nu^{\sigma\sigma}(-\vec{k}_1)\, b^{\dagger}_{\vec{k}+\vec{q}+\vec{k}_1\sigma}\, b_{\vec{k}-\sigma}\\
&+ \epsilon_{\vec{k}}\, b^{\dagger}_{\vec{k}+\vec{q}\sigma}\, b_{\vec{k}-\sigma} - \sum_{\vec{k}_1} \epsilon_{\vec{k}_1}\, b^{\dagger}_{\vec{k}+\vec{q}\sigma}\, b_{\vec{k}_1-\sigma}\,\nu^{\sigma-\sigma}_{(\vec{k}_1-\vec{k})} + \sum_{\vec{k}_1} \epsilon_{\vec{k}_1}\, b^{\dagger}_{\vec{k}+\vec{q}\sigma}\, b_{\vec{k}_1\sigma}\,\nu^{\sigma-\sigma}(\vec{k}_1-\vec{k})\\
&+ 2\sum_{\vec{k}_1} K_{\vec{k}_1}\, b^{\dagger}_{\vec{k}+\vec{q}\sigma}\, b_{\vec{k}+\vec{k}_1-\sigma}\,\nu^{\sigma_1\sigma_1}(\vec{k}_1) + 4\sum_{\vec{k}_1} \tilde{J}_{\vec{k}_1}\, b^{\dagger}_{\vec{k}+\vec{q}\sigma}\, b_{\vec{k}+\vec{k}_1\sigma}\,\nu^{\sigma-\sigma}(\vec{k}_1) - 2\sum_{\vec{k}_1} \tilde{J}_{\vec{k}_1}\, b^{\dagger}_{\vec{k}+\vec{q}\sigma}\, b_{\vec{k}+\vec{k}_1-\sigma}\,\nu^{\sigma\sigma}(\vec{k}_1) \quad .
\end{aligned}
$$

The right-hand side of the above equation contains many terms so that a rigorous treatment is difficult. We retain only a few terms by making an ansatz for the spin-density operator,

$$
\nu^{\sigma\sigma'}(\vec{k}) = \nu^{\sigma\sigma'}(0)\,\delta_{\vec{k},0} + \nu^{\sigma\sigma'}(\vec{q})\,\delta_{\vec{k},q} \quad , \qquad (44)
$$

and replacing the operators $b^{\dagger}_{\vec{k}\sigma} b_{\vec{k}'\sigma'}$ which are multiplied by $\nu^{\sigma-\sigma}(\vec{q})$ or $\nu^{\sigma-\sigma}_{\vec{k}}(\vec{q})$, by $\langle b^{\dagger}_{\vec{k}\sigma} b_{\vec{k}\sigma}\rangle\,\delta_{\vec{k}\vec{k}'}\,\delta_{\sigma\sigma'}$. This approximation is very similar to the random-phase approximation in the weak-intra-atomic-interaction theory. In this approximation, the equation of motion (43) becomes

$$
\begin{aligned}
\omega\langle\langle \nu^{-+}_{\vec{k}}(\vec{q});\ \nu^{+-}(-\vec{q})\rangle\rangle_{\omega} = &\frac{1}{2\pi}\,\langle [\nu^{-+}_{\vec{k}}(\vec{q}),\ \nu^{+-}(-\vec{q})]_-\rangle\\
&+ A^{-+}_{\vec{k}\vec{q}}\,\langle\langle \nu^{-+}_{\vec{k}}(\vec{q});\ \nu^{+-}(-\vec{q})\rangle\rangle_{\omega}\\
&+ \frac{B^{-+}_{\vec{k}\vec{q}}}{N}\sum_{\vec{k}_1}\langle\langle \nu^{-+}_{\vec{k}_1}(\vec{q});\ \nu^{+-}(\vec{q})\rangle\rangle_{\omega} \quad , \qquad (45)
\end{aligned}
$$

where

$$
\begin{aligned}
A^{-+}_{\vec{k}\vec{q}} = &\epsilon_{\vec{k}}(1 - \langle \nu^{--}(0)\rangle) - \epsilon_{\vec{k}+\vec{q}}(1 - \langle \nu^{++}(0)\rangle)\\
&+ 4\tilde{J}_0 \textstyle\sum_{\sigma}\langle \nu^{\sigma\sigma}(0)\rangle \quad , \qquad (46)
\end{aligned}
$$

$$
B^{-+}_{\vec{k}\vec{q}} = (\epsilon_{\vec{k}+\vec{q}} + 4\tilde{J}_{\vec{q}})\langle b^{\dagger}_{\vec{k}+\vec{q}-} b_{\vec{k}+\vec{q}-}\rangle - (\epsilon_{\vec{k}} + 4\tilde{J}_{\vec{q}})\langle b^{\dagger}_{\vec{k}+} b_{\vec{k}+}\rangle \quad . \qquad (47)
$$

The first term on the right-hand side of Eq. (45) is given by

$$
\langle [\nu^{-+}_{\vec{k}}(\vec{q}),\ \nu^{+-}(-\vec{q})]_-\rangle
$$

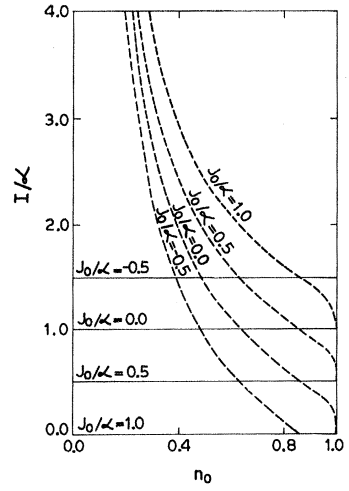

FIG. 2. Phase boundaries between different magnetic states in the weak-interaction theory. Dashed curves denote the phase boundaries between the para- and antiferromagnetic states. Solid lines represent the boundary between the para- and ferromagnetic states.

$$= \langle b^{\dagger}_{\vec{k}+\vec{q}\,-} b_{\vec{k}+\vec{q}\,-}\rangle - \langle b^{\dagger}_{\vec{k}+} b_{\vec{k}+}\rangle - \sum_{\vec{k}_1} [\langle b^{\dagger}_{\vec{k}_1+} \nu^{++}(\vec{k}-\vec{k}_1) b_{\vec{k}+}\rangle - \langle b^{\dagger}_{\vec{k}+\vec{q}\,-} \nu^{--}(\vec{k}_1-\vec{k}) b_{\vec{k}_1+\vec{q}\,-}\rangle] .$$

The correlation function inside the square brackets corresponds to the creation of two holes and two electrons of the same spin simultaneously. We assume that there is a very small probability of occurrence of such processes and we neglect these terms. The equation of motion (45) takes the form

$$(\omega - A^{+}_{\vec{k}\vec{q}})\langle\langle \nu^{+}_{\vec{k}}(\vec{q}); \nu^{+-}(-\vec{q})\rangle\rangle_{\omega} = (\langle b^{\dagger}_{\vec{k}+\vec{q}\,-} b_{\vec{k}+\vec{q}\,-}\rangle - \langle b^{\dagger}_{\vec{k}+} b_{\vec{k}+}\rangle)/2\pi + (B^{+}_{\vec{k}\vec{q}}/N)\sum_{\vec{k}} \langle\langle \nu^{+}_{\vec{k}}(\vec{q}); \nu^{+-}(-\vec{q})\rangle\rangle_{\omega} . \quad (48)$$

When we divide both sides of the above equation by $(\omega - A^{+}_{\vec{k}\vec{q}})$ and sum of over $\vec{k}$, we get the Green's function $\langle\langle \nu^{-+}(\vec{q}); \nu^{+-}(-\vec{q})\rangle\rangle_{\omega}$ and hence the dynamical susceptibility

$$\chi_{-+}(\vec{q}, \omega) = g^2\mu_B^2 \sum_{\vec{k}} \frac{\langle b^{\dagger}_{\vec{k}+\vec{q}\,-} b_{\vec{k}+\vec{q}\,-}\rangle - \langle b^{\dagger}_{\vec{k}+} b_{\vec{k}+}\rangle}{\omega + A^{+}_{\vec{k}\vec{q}}} \Bigg/ \left(1 + \frac{1}{N}\sum_{\vec{k}} \frac{B^{+}_{\vec{k}\vec{q}}}{\omega + A^{+}_{\vec{k}\vec{q}}}\right) . \quad (49)$$

The averages $\langle b^{\dagger}_{\vec{k}\sigma} b_{\vec{k}\sigma}\rangle$ can be obtained from the knowledge of the one-particle Green's function $\langle\langle b_{\vec{k}\sigma}; b^{\dagger}_{\vec{k}\sigma}\rangle\rangle_{\omega}$ $(\eta = +1)$. Recently, Richmond and Sewell[10] have obtained this Green's function within the approximations which we have used to derive the dynamical susceptibility $\chi_{-+}(\vec{q}, \omega)$. They obtained

$$\langle\langle b_{\vec{k}\sigma}; b^{\dagger}_{\vec{k}\sigma}\rangle\rangle_{\omega} = \frac{1}{2\pi}(1 - \langle \nu^{-\sigma-\sigma}(0)\rangle) \Bigg/ \left(\omega - \epsilon_{\vec{k}}(1 - \langle \nu^{-\sigma-\sigma}(0)\rangle) - 2K_0\nu_0 - 2\tilde{J}_0\sigma\sum_{\sigma}\sigma\langle \nu^{\sigma\sigma}(0)\rangle\right) , \quad (50)$$

where $\nu_0 = \sum_{\sigma}\langle \nu^{\sigma\sigma}(0)\rangle$ is the number of electrons per atom. From the poles of the Green's function (50), the single-particle energies are given by

$$\omega_{\vec{k}\sigma} = \epsilon_{\vec{k}}(1 - \langle \nu^{-\sigma-\sigma}(0)\rangle) + 2K_0\nu_0 + 2\tilde{J}_0\sigma\sum_{\sigma}\sigma\langle \nu^{\sigma\sigma}(0)\rangle . \quad (51)$$

In Eq. (51) the factor $(1 - \langle \nu^{-\sigma-\sigma}(0)\rangle)$ represents a "band narrowing" due to restrictions imposed on the electronic motion by the exclusion of doubly occupied atomic states, while the terms $2K_0\nu_0$ and $2\tilde{J}_0\sigma\sum_{\sigma}\sigma\langle \nu^{\sigma\sigma}(0)\rangle$ represent additional contributions to the energy of the electron due to interatomic Coulomb and exchange interactions. When we substitute the value of the Green's function $\langle\langle b_{\vec{k}\sigma}; b^{\dagger}_{\vec{k}\sigma}\rangle\rangle_{\omega}$ in Eq. (A3) we get the average as

$$\langle b^{\dagger}_{\vec{k}\sigma} b_{\vec{k}\sigma}\rangle = (1 - \langle \nu^{-\sigma-\sigma}(0)\rangle) f(\epsilon_k(1 - \langle \nu^{-\sigma-\sigma}(0)\rangle) + 2K_0\nu_0 + 2\tilde{J}_0\sigma\sum_{\sigma}\sigma\langle \nu^{\sigma\sigma}(0)\rangle) . \quad (52)$$

From Eq. (35) we have $\langle Q\rangle = \langle Q_0\rangle$, where on the left-hand side the ensemble average is taken over the states in space S_0 while on the right-hand side the average is over the states in subspace S. To compare the results of this section to the results of weak-interaction theory, hereafter we shall replace the ensemble average of the operators in subspace S by the ensemble average of the operators in space S_0.

In the limit of zero bandwidth, the dynamical susceptibility (49) reduces to

$$\chi_{-+}(\vec{q}, \omega) = g^2\mu_B^2 \sum_{\sigma}\sigma\langle n^{\sigma\sigma}(0)\rangle / [(J_0 - J_{\vec{q}})\sum_{\sigma}\sigma\langle n^{\sigma\sigma}(0)\rangle - \omega] . \quad (53)$$

This is an expression which one obtains for a Heisenberg model under the random-phase approximation.[22] It should be noted that the dynamical susceptibility (16) obtained in the weak-intra-atomic-interaction theory also reduces to (53) in the limit of zero bandwidth. Thus, in the zero-bandwidth limit both weak- and strong-interaction theories are equivalent.

For a system with a small number of electrons $(n_0 \ll 1)$ and $|J_{\vec{q}}| \gg \frac{1}{2}\alpha$, Eq. (49) takes the form

$$\chi_{-+}(\vec{q}, \omega) = -g^2\mu_B^2 \sum_{\vec{k}} \frac{\langle a^{\dagger}_{\vec{k}+\vec{q}\,-} a_{\vec{k}+\vec{q}\,-}\rangle - \langle a^{\dagger}_{\vec{k}+} a_{\vec{k}+}\rangle}{-\omega - \epsilon_{\vec{k}} + \epsilon_{\vec{k}+\vec{q}} + J_0\sum_{\sigma}\sigma\langle n^{\sigma\sigma}(0)\rangle} \Bigg/ \left(1 + \frac{J_{\vec{q}}}{N}\sum_{\vec{k}} \frac{\langle a^{\dagger}_{\vec{k}+\vec{q}\,-} a_{\vec{k}+\vec{q}\,-}\rangle - \langle a^{\dagger}_{\vec{k}+} a_{\vec{k}+}\rangle}{-\omega - \epsilon_{\vec{k}} + \epsilon_{\vec{k}+\vec{q}} + J_0\sum_{\sigma}\sigma\langle n^{\sigma\sigma}(0)\rangle}\right) , \quad (54)$$

and (52) becomes

$$\langle a^{\dagger}_{\vec{k}\sigma} a_{\vec{k}\sigma}\rangle = f(\epsilon_{\vec{k}} + 2V_0 n_0 - J_0\langle n^{\sigma\sigma}(0)\rangle) . \quad (55)$$

Equations (54) and (55) are the same as Eqs. (16) and (18) provided $I + J_{\vec{q}}$ is replaced by $J_{\vec{q}}$. This similarity between strong- and weak-intra-atomic-interaction theories is very similar to that pointed out by Kanamori.[23] He has shown that for a system of electrons interacting by strong intra-atomic interaction, the random-phase approximation is good provided the density of electrons is small and the bare intra-atomic interaction is replaced by some effective intra-atomic interaction.

From Eqs. (49) and (52) the static paramagnetic susceptibilities $\chi(00)$ and $\chi(\vec{Q}, 0)$ needed to discuss the instability of the paramagnetic states against the ferro- and the antiferromagnetic states, respectively, are given by

$$\chi(00) = g^2\mu_B^2\beta(1 - \tfrac{1}{2}n_0)^2\sum_{\vec{k}} \Gamma_{\vec{k}}(00) \Bigg/ \left(1 - n_0 + \frac{\beta(1 - \frac{1}{2}n_0)^2}{n}\sum_{\vec{k}}(\epsilon_{\vec{k}} - J_0)\Gamma_{\vec{k}}(00)\right) , \quad (56)$$

where

$$\Gamma_{\vec{k}}(00) = f(\epsilon_{\vec{k}}(1 - \tfrac{1}{2}n_0) + 2K_0 n_0)$$

$$\times[1-f(\epsilon_{\vec{k}}(1-\tfrac{1}{2}n_0)+2K_0n_0)]\ , \quad (57)$$

and

$$\chi(\vec{Q},0)=g^2\mu_B^2\,[\tfrac{1}{4}(2-n_0)]\Gamma(\vec{Q},0)\Big/\left(1-n_0+\frac{(2-n_0)J_0}{4N}\,\Gamma(\vec{Q},0)\right)\ , \quad (58)$$

where

$$\Gamma(\vec{Q},0)=\sum_{\vec{k}\sigma}\sigma f(-\sigma\epsilon_{\vec{k}}(1-\tfrac{1}{2}n_0)+2K_0n_0)/\epsilon_{\vec{k}}\ . \quad (59)$$

The chemical potential μ is determined by

$$\frac{n_0}{2-n_0}=\frac{1}{N}\sum_{\vec{k}} f(\epsilon_{\vec{k}}(1-\tfrac{1}{2}n_0)+2K_0n_0)\ . \quad (60)$$

A. Instability of Paramagnetic State against Ferromagnetic States

At the absolute zero of temperature, the denominator of the dynamical susceptibility [Eq. (56)] gives the criterion for the instability of the paramagnetic state:

$$1-n_0+[\mu-2K_0n_0-J_0(1-\tfrac{1}{2}n_0)]\,\rho\left(\frac{\mu-2K_0n_0}{1-\frac{1}{2}n_0}\right)\leq 0\ . \quad (61)$$

In the absence of interatomic interactions, the inequality (61) has been derived recently by Sakurai[8] and Hubbard and Jain[9] in the limit of strong-intra-atomic interaction. Sakurai has analyzed the instability leading to the ferromagnetic state, and has reached the following conclusions:

(i) The paramagnetic state is unstable for a system with a small number of electrons if the density of states at the bottom of the band is large enough (for a nearly filled electron band, the high density of states at the top of the band is required for the instability).

(ii) When the narrowed band is more than half-filled ($\mu\geq 0$), the paramagnetic state is always more stable than the ferromagnetic state.

In the presence of interatomic interactions both the conclusions of Sakurai are modified.

(i) When the number of electrons per atom is small ($n_0\ll 1$) the inequality (61) reduces to

$$1+(\mu-2K_0n_0-J_0)\,\rho(\mu-2K_0n_0)\leq 0\ . \quad (62)$$

For a small number of electrons per atom, the Fermi level lies below the middle of the band $\omega_{\vec{k}\sigma}$ (i.e., $\mu<2K_0n_0$); therefore inequality (62) can be satisfied for the high density of states at the bottom of band if $J_0>\mu-2K_0n_0$. On the other hand, if $J_0<\mu-2K_0n_0$, the inequality is never satisfied whatever may be the value of density of states.

(ii) For $n_0=\frac{2}{3}$ the band is half-filled, because in that case Eq. (60) is satisfied for $\mu=2K_0n_0$. For a more than half-filled band (i.e., $n_0>\frac{2}{3}$ or $\mu-2K_0n_0>0$), the paramagnetic state cannot be unstable if $\mu-2K_0n_0>J_0(1-\frac{1}{2}n_0)$, but if $\mu-2K_0n_0<J_0(1-\frac{1}{2}n_0)$ the paramagnetic state may become unstable for large values of density of states.

To be more specific, we shall discuss the inequality (61) for square density of states. In this case, Eq. (60) gives the chemical potential

$$\mu=2K_0n_0+\tfrac{1}{2}\alpha(\tfrac{3}{2}n_0-1)\ , \quad (63)$$

hence the inequality (61) becomes

$$J_0/\alpha>0.5\ . \quad (64)$$

At finite temperatures for zero bandwidth, Eq. (56) with the help of Eq. (60) gives the Curie-Weiss law given by Eq. (25) with $C=Ng^2\mu_B^2n_0/2k_B$ and $T_c=J_0n_0/2k_B$. When we compare the values of C and T_c with the values obtained in the weak-intra-atomic-interactions theory for $I=0$, we see that both the Curie constant C and the Curie temperature T_c are enhanced in the strong-intra-atomic-interaction theory. Recently, a similar conclusion has been reached by Mattuck[24] who has shown that, in the Hubbard model, correlation effects enhance the critical temperature.

To study the instability of the paramagnetic state for a finite bandwidth, we restrict our analysis to the half-filled narrowed band ($n_0=\frac{2}{3}$ and $\mu=2K_0n_0$). From Eq. (56) the instability of the paramagnetic state is given by

$$1+\frac{4\beta}{3N}\sum_{\vec{k}}(\epsilon_{\vec{k}}-J_0)(e^{2\beta\epsilon_{\vec{k}}/3}+1)^{-2}\leq 0\ . \quad (65)$$

For square density of states it gives the transition temperature

$$T_c=\tfrac{2}{3}\alpha\Big/4k_B\tanh^{-1}\left(\frac{\frac{2}{3}\alpha}{\frac{4}{3}J_0}\right)\ . \quad (66)$$

This result is the same as the result (29) obtained in the weak-interaction theory provided one replaces α by $\frac{2}{3}\alpha$ and $(I+J_0)$ by $\frac{4}{3}J_0$ in Eq. (29).

B. Instability of Paramagnetic State against Antiferromagnetic State

At the absolute zero of temperature from Eq. (58), the condition for the instability of the paramagnetic state is given by

$$1-n_0+\tfrac{1}{4}(2-n_0)J_0\sum_{\sigma}\sigma\int d\epsilon\,\frac{\eta(\epsilon)}{\epsilon}\times\theta(\mu-2K_0n_0+\sigma\epsilon(1-\tfrac{1}{2}n_0)\leq 0\ .$$

For the square density of states it gives

$$\frac{J_0}{\alpha}\leq(n_0-1)\Big/(1-\tfrac{1}{2}n_0)\ln\left|\frac{2-n_0}{3n_0-2}\right|\ . \quad (67)$$

The boundary line, given by the equality sign in (67), between the para- and the antiferromagnetic states is shown in Fig. 3. We have also shown the line $J_0/\alpha=0.5$ given by (64) which gives the bound-

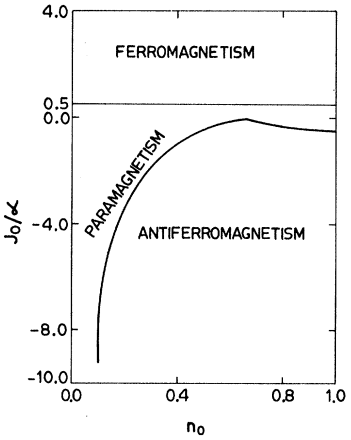

FIG. 3. Phase boundaries between different magnetic states in strong-interaction theory.

ary line between para- and ferromagnetic states. For $0 < J_0/\alpha < 0.5$, the paramagnetic state is stable for all values of n_0. This can be compared with the result of the weak-interaction theory (for $I = 0$) where the paramagnetic state is stable for $0 < J_0/\alpha < 1.0$.

At finite temperatures for zero bandwidth, Eq. (58) gives the Curie-Weiss law given by Eq. (32) with $C = g^2\mu_B^2 N n_0/2k_B$ and $T_N = -J_0 n_0/2k_B$. A negative sign in the expression for the Néel temperature shows that for antiferromagnetism to exist J_0 must be negative. When we compare T_N with the T_N obtained in weak-interaction theory for $I = 0$, we see that, like the Curie temperature, the Néel temperature has also been enhanced because of strong correlations. For finite bandwidth, we restrict our analysis to the half-filled narrowed band ($n_0 = \frac{2}{3}$). In this case, instability condition takes the form

$$1 - \frac{4J_0}{3N}\sum_{\vec{k}} \frac{\tanh(\frac{1}{2}\beta E_{\vec{k}})}{E_{\vec{k}}} \leq 0, \tag{68}$$

where $E_{\vec{k}} = \frac{2}{3}\epsilon_{\vec{k}}$. Equation (68) reduces to Eq. (34) if one replaces $\frac{4}{3}J_0$ by $I - J_0$ in Eq. (68) and $E_{\vec{k}}$ by $\epsilon_{\vec{k}}$. Thus, the results for the half-filled band, both in weak-interaction theory ($n_0 = 1$) and strong-interaction theory ($n_0 = \frac{2}{3}$) are of the same type.

C. Spin-Wave Excitation

The dispersion relations for the spin waves are determined by the poles of the dynamical susceptibility, i.e., from

$$1 - \frac{1}{N}\sum_{\vec{k}} \frac{B^{-+}_{\vec{k}\vec{q}}}{\omega + A^{-+}_{\vec{k}\vec{q}}} = 0 . \tag{69}$$

This equation has solutions corresponding to individual modes, or the Stoner excitations, as well as the spin-wave modes. Stoner excitations are given by

$$\omega_s + A^{-+}_{\vec{k}\vec{q}} = 0 . \tag{70}$$

When we substitute the value of $A^{-+}_{\vec{k}\vec{q}}$ from Eq. (46) we get

$$\omega_s = (\epsilon_{\vec{k}+\vec{q}} - \epsilon_{\vec{k}})(1 - \tfrac{1}{2}n_0) + [J_0 - \tfrac{1}{2}(\epsilon_{\vec{k}} + \epsilon_{\vec{k}+\vec{q}})]\sum_\sigma \sigma \langle n^{\sigma\sigma}(0)\rangle . \tag{71}$$

For $q = 0$, it gives

$$\omega_s = (J_0 - \epsilon_{\vec{k}})\sum_\sigma \sigma \langle n^{\sigma\sigma}(0)\rangle . \tag{72}$$

It shows that if $J_0 < \frac{1}{2}\alpha$, there is no gap in the spectrum of Stoner excitations, and hence, in this region spin waves with infinite lifetime do not exist. This is consistent with our previous conclusions for the stability of the paramagnetic state against the ferromagnetic state. We have shown that for square density of states, the ferromagnetic state is unstable for $J_0/\alpha < 0.5$. When $J_0/\alpha > 0.5$, a gap in the spectrum of Stoner excitations occurs at $\vec{q} = 0$, and for small values of $\vec{q}$ we get spin waves with infinite lifetime. Let us assume that $J_0 \gg \alpha/2$, and ω satisfies the condition

$$J_0 \sum_\sigma \sigma \langle n^{\sigma\sigma}(0)\rangle \gg \left| (\epsilon_{\vec{k}} - \epsilon_{\vec{k}+\vec{q}})(1 - \tfrac{1}{2}n_0)\right| , \omega .$$

Under the above assumptions, for small $\vec{q}$ we get the spin-wave dispersions from Eq. (69)

$$\omega = (J_0 - J_{\vec{q}})\langle S_0^z\rangle + \frac{1 - n_0/2}{2N\langle S_0^z\rangle} \times \sum_{\vec{k}} (\langle a^\dagger_{\vec{k}+}a_{\vec{k}+}\rangle + \langle a^\dagger_{\vec{k}-}a_{\vec{k}-}\rangle)(\vec{q}\cdot\nabla_{\vec{k}})^2\epsilon_{\vec{k}} - \frac{(1 - n_0/2)^2}{2NJ_0\langle S_0^z\rangle^2} \times \sum_{\vec{k}} (\langle a^\dagger_{\vec{k}+}a_{\vec{k}+}\rangle - \langle a^\dagger_{\vec{k}+\vec{q}-}a_{\vec{k}+\vec{q}-}\rangle) \times (\vec{q}\cdot\nabla_{\vec{k}}\epsilon_{\vec{k}})^2 + O(q^4), \tag{73}$$

where $\langle S_0^z\rangle = \sum_\sigma \sigma \langle n^{\sigma\sigma}(0)\rangle$. Here we have assumed that $\epsilon_{\vec{k}} = \epsilon_{-\vec{k}}$. For a small number of electrons per atom ($n_0 \ll 1$), Eq. (73) reduces to an expression obtained within the random-phase approximation[13] if one replaces J_0 by $(I + J_0)$ in the third term on its right-hand side.

V. CONCLUSIONS

We have discussed the dynamical susceptibility for a model Hamiltonian which takes into account the interatomic Coulomb and exchange interactions over the Hubbard Hamiltonian. For the weak-intra-atomic interaction we have obtained an expression for the dynamical susceptibility which is very similar to that of Englert and Antonoff.[13] It is found that in the presence of the interatomic interactions, the results of the Hubbard model are considerably modified. For example, for the square density of states at absolute zero according to the Hubbard model in a half-filled band ($n_0 = 1$), the paramagnetic state is always unstable against the ferro- and the antiferromagnetic states. In the presence of the interatomic interactions, we find that it is possible to have a paramagnetic ground state for $J_0/\alpha > 0$.

At finite temperature for the zero bandwidth the Curie-Weiss law is obtained. It is found that for positive J_0 the Curie temperature obtained from the Hubbard model increases while the Néel temperature decreases. For negative J_0 these conclusions are reversed.

In the strong-intra-atomic-interaction theory we have obtained an expression for the dynamical susceptibility which reduces to an expression obtained in the weak-intra-atomic-interaction theory for $I=0$, when the density of electrons is small ($n_0 \ll 1$) and $J_{\vec{q}} \gg \alpha/2$. Here also the results of the Hubbard model are modified. For example, at absolute zero the Hubbard model predicts that for the square density of states the paramagnetic state is always more stable than the ferro- and the antiferromagnetic states. Here we find that for $J_0/\alpha > 0.5$ the ferromagnetic state is stable for all values of n_0, for $0 < J_0/\alpha < 0.5$ the paramagnetic state is stable for all values of n_0, and for $J_0/\alpha < 0$ both the para- and antiferromagnetic states are stable in the regions shown in Fig. 3. Whatever may be the density of states, the Hubbard model predicts that for $n_0 > \frac{2}{3}$, the paramagnetic state is more stable than the ferromagnetic state. Here we find that the paramagnetic state is unstable against the ferromagnetic states for higher density of states if $(\mu - 2K_0 n_0) < J_0(1 - \frac{1}{2}n_0)$. For a small number of electrons, the Hubbard model predicts that the paramagnetic state is unstable against the ferromagnetic state if the density of states at the bottom of the band is large. In the presence of interatomic interactions, and if $J_0 < (\mu - 2K_0 n_0)$, the paramagnetic state is always stable whatever may be the value of the density of states. Finite-temperature theory shows that for the zero-bandwidth case, Curie and Néel temperatures have higher values compared to the weak-intra-atomic-interaction theory for $I=0$. For the square density of states and for a half-filled narrowed band ($n_0 = \frac{2}{3}$), the expressions for Curie and Néel temperatures come out to be very similar to those obtained in weak-interaction theory for $n_0 = 1$. For $J_0/\alpha > 0.5$, spin-wave dispersion relations are found to be very similar to those obtained in weak-intra-atomic-interaction theory.

Thus we see that interatomic interactions play an important role in the magnetic properties of the system. Our treatment is approximate and qualitative, but it gives some insight into the effect of interatomic interactions and reveals that in any complete theory of magnetism, interatomic interactions should not be neglected.

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APPENDIX

The purpose of this Appendix is to evaluate the average $\langle a^\dagger_{\vec{k}\sigma} a_{\vec{k}\sigma}\rangle$ within the Hartree-Fock approximation. $\langle a^\dagger_{\vec{k}\sigma} a_{\vec{k}\sigma}\rangle$ can be obtained from the one-particle Green's function $\langle\langle a_{\vec{k}\sigma}; a^\dagger_{\vec{k}\sigma}\rangle\rangle_\omega$ ($\eta = +1$). The equation of motion for this Green's function is

$$
\begin{aligned}
&(\omega - \epsilon_{\vec{k}})\langle\langle a_{\vec{k}\sigma}; a^\dagger_{\vec{k}\sigma}\rangle\rangle_\omega \\
&= \frac{1}{2\pi} + \frac{I}{N}\sum_{\vec{k}_1\vec{k}_2}\langle\langle a^\dagger_{\vec{k}_1 -\sigma} a_{\vec{k}+\vec{k}_1-\vec{k}_2 -\sigma} a_{\vec{k}_2\sigma}; a^\dagger_{\vec{k}\sigma}\rangle\rangle_\omega \\
&+ \frac{1}{N}\sum_{\vec{k}_1\vec{k}_2;\sigma_1} V_{\vec{k}_1}\langle\langle a^\dagger_{\vec{k}_2\sigma_1} a_{\vec{k}_1+\vec{k}_2\sigma_1} a_{\vec{k}-\vec{k}_1\sigma}; a^\dagger_{\vec{k}\sigma}\rangle\rangle_\omega \\
&+ \frac{1}{N}\sum_{\vec{k}_1\vec{k}_2;\sigma_1} J_{\vec{k}_1}\langle\langle a^\dagger_{\vec{k}_2\sigma_1} a_{\vec{k}-\vec{k}_1\sigma_1} a_{\vec{k}_1+\vec{k}_2\sigma}; a^\dagger_{\vec{k}\sigma}\rangle\rangle_\omega . \qquad \text{(A1)}
\end{aligned}
$$

In the Hartree-Fock approximation, the higher-order Green's functions are decoupled as

$$
\begin{aligned}
\langle\langle a^\dagger_{\vec{k}_1\sigma_1} a_{\vec{k}_2\sigma_1} a_{\vec{k}_3\sigma}; a^\dagger_{\vec{k}\sigma}\rangle\rangle_\omega \simeq \langle n_{\vec{k}_1\sigma_1}\rangle [\delta_{\vec{k}_1\vec{k}_2}\langle\langle a_{\vec{k}_3\sigma}; a^\dagger_{\vec{k}\sigma}\rangle\rangle_\omega \\
- \delta_{\vec{k}_1\vec{k}_3}\delta_{\sigma_1\sigma}\langle\langle a_{\vec{k}_2\sigma}; a^\dagger_{\vec{k}\sigma}\rangle\rangle_\omega] .
\end{aligned}
$$

In this approximation, the equation of motion (A1) gives the Green's function $\langle\langle a_{\vec{k}\sigma}; a^\dagger_{\vec{k}\sigma}\rangle\rangle_\omega$ as

$$
\begin{aligned}
\langle\langle a_{\vec{k}\sigma}; a^\dagger_{\vec{k}\sigma}\rangle\rangle_\omega = \frac{1/2\pi}{\omega - \epsilon_{\vec{k}} - I\langle n^{-\sigma -\sigma}(0)\rangle - V_0 n_0 + J_0\langle n^{\sigma\sigma}(0)\rangle} \\
- \frac{1}{N}\sum_{\vec{k}_1} V_{\vec{k}-\vec{k}_1}\langle a^\dagger_{\vec{k}_1 -\sigma} a_{\vec{k}_1 -\sigma}\rangle .
\end{aligned}
$$

If we neglect the last term in the denominator, as we have done in Sec. III, we get

$$
\langle\langle a_{\vec{k}\sigma}; a^\dagger_{\vec{k}\sigma}\rangle\rangle_\omega = \frac{1/2\pi}{\omega - \epsilon_{\vec{k}} - I\langle n^{-\sigma -\sigma}(0)\rangle - V_0 n_0 + J_0\langle n^{\sigma\sigma}(0)\rangle} . \qquad \text{(A2)}
$$

With the help of the spectral theorem[14]

$$
\langle BA\rangle = i\lim_{\epsilon\to 0^+}\int_{-\infty}^{\infty}\frac{\langle\langle A; B\rangle\rangle_{\omega+i\epsilon} - \langle\langle A; B\rangle\rangle_{\omega-i\epsilon}}{e^{\beta(\omega-\mu)}+1}\, d\omega , \qquad \text{(A3)}
$$

the average $\langle a^\dagger_{\vec{k}\sigma} a_{\vec{k}\sigma}\rangle$ can be expressed as

$$
\langle a^\dagger_{\vec{k}\sigma} a_{\vec{k}\sigma}\rangle = f(\epsilon_{\vec{k}} + I\langle n^{-\sigma -\sigma}(0)\rangle + V_0 n_0 - J_0\langle n^{\sigma\sigma}(0)\rangle) . \qquad \text{(A4)}
$$

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Universality of Critical Correlations in the Three-Dimensional Ising Ferromagnet*

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Evidence from exact enumeration series is presented to support the hypothesis that the functional form of spin-spin correlations for three-dimensional zero-field Ising ferromagnets in their high-temperature critical region is independent of lattice and spin magnitude.

I. INTRODUCTION

There is strong evidence, both theoretical[1] and experimental,[2] that the critical properties of a system undergoing a thermodynamic phase transition depend crucially on both the spatial dimensionality of the system and the symmetry of the ordering in the ordered phase.[3] In order to develop a first-principles theory of the critical region, it is important to know within these restrictions, i.e., for fixed dimensionality and symmetry, just how universal critical behavior is.[4]

Are critical properties independent of such details as spin magnitude and lattice type, or are they not? Results based on exact perturbation series for magnetic models strongly suggest that the critical exponents are independent of lattice type.[1,5] The evidence that the exponents do not depend on spin magnitude is somewhat weaker but still convincing.[6,7] The logically next and stronger hypothesis is that the functional forms of the equation of state and of the critical correlations are universal. Recent series evidence suggests that the equation of state is lattice independent both above and below T_c.[8] We present below evidence that the critical correlations are universal with respect to lattice type, and we investigate their dependence on spin magnitude.

II. MOMENT-RATIO TEST

It is generally believed that the critical spin-spin correlation function of the three-dimensional Ising model in zero magnetic field has the spherically symmetrical scaling form[9]

$$\Gamma(\vec{r}, T) \equiv \langle S_{\vec{r}}^z S_{\vec{0}}^z \rangle - \langle S_{\vec{r}}^z \rangle \langle S_{\vec{0}}^z \rangle = (a/r)^{1+\eta} D(\kappa r) , \qquad (1)$$

where $r = |\vec{r}|$, the inverse correlation length $\kappa(T) \equiv \xi^{-1}(T) = \kappa_0 \epsilon^{\nu}$, $\epsilon \equiv 1 - T_c/T$, η and ν are the conventionally defined[1] critical indices, and T_c, κ_0, and a are constants known to depend on both lattice type and spin magnitude. We assume that (1) holds for r large and κ small.[10] This paper examines the universality of the function $D(x = \kappa r)$ for $T \geq T_c$.

Only for the fcc lattice and $S = \frac{1}{2}$ are existing series data good enough to infer D directly.[10] For other situations we probe D by examining the spherical moments $u_n \equiv \sum_{\vec{r} \neq 0} r^n \Gamma(\vec{r}, T)$. As $\kappa \to 0$, the correlation length becomes longer than any fixed lattice spacing and one may convert the divergent part of the sum to an integral. Using (1), one finds[11]

$$\mu_n(T) = 4\pi a^{1+\eta} U_n \kappa^{-n-2+\eta} + (\text{less-singular terms}), \qquad (2)$$