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Application of the Roth Decoupling Scheme to the Kondo Problem*

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A self-consistent treatment of the Kondo problem as described by the s-d exchange model is presented. The treatment is based on the Roth prescription for linearizing the equations of motion for the Green's functions. The result for the t matrix is the same as in the Nagaoka theory. The treatment, however, yields different results for higher-order thermal averages. Some difficulties associated with the Roth scheme are also discussed.

I. INTRODUCTION

The Kondo problem as described by the s-d exchange model has been treated by Nagaoka[1] using the method of decoupled equations of motion for Green's functions. Although the Nagaoka treatment is attractive from the viewpoint that the formalism is simple and familiar, the key approximation is a somewhat arbitrary decoupling procedure. The heuristic justification for the decoupling approximation is that it takes into account the correlation between spins of the impurity and conduction elec-

trons. At high temperatures, the decoupling scheme has been demonstrated[2] to be essentially the same as the perturbation expansion.

In this paper the Roth[3] prescription for decoupling equations of motion for Green's functions is applied to this s-d exchange model. The basic approximation in the Roth scheme is the choice of a restricted basis set of operators. Our choice is motivated by the same physical requirement as the decoupling approximation of the Nagaoka theory; namely, any nontrivial treatment must take into account the correlation between spins of the impurity and the conduction electrons. Our choice of a basis set of operators appears to be the simplest nontrivial choice possible. By our choice of a basis set we make all the basic approximations of the Nagaoka theory except for the details of the decoupling procedure. The reasons for this treatment of the Kondo problem based on the Roth scheme are twofold. One hopes to obtain further understanding of the Nagaoka decoupling procedure. Also, the Kondo Hamiltonian provides a nontrivial problem for the application of the Roth procedure. Our treatment illustrates some difficulties associated with this method.

In Sec. II the Nagaoka theory is briefly reviewed. The Roth decoupling scheme is outlined in Sec. III and applied to the Kondo problem for a particular choice of basis operators. The resulting energy and normalization matrices are given. These matrices are used to construct the required Green's functions in Sec. IV. A self-consistent solution for the t matrix is obtained which is identical to the t matrix obtained by the Nagaoka treatment. In Sec. V, the results are discussed.

II. REVIEW OF NAGAOKA THEORY

Nagaoka's theory[1,2] treats the Kondo problem as described by the so-called s-d exchange model. The model Hamiltonian is given by

$$H=\sum_k \epsilon_k C^\dagger_{k\mu} C_{k\mu} - \frac{J}{2N}\sum_{kk'} \vec{\sigma}_{\mu\mu'}\cdot\vec{S}\, C^\dagger_{k\mu} C_{k'\mu'} \quad , \tag{1}$$

where $C^\dagger_{k\mu}$ and $C_{k\mu}$ are the creation and annihilation operators of the conduction electron with momentum k and spin μ, ϵ_k is its band energy measured from the Fermi energy, and $\vec{S}$ is the spin operator associated with the impurity located at the origin.

Here $\vec{\sigma}_{\mu\mu'}$ denotes the $\mu\mu'$ component of the Pauli matrix, and summation of repeated spin indices is understood. J is the exchange coupling constant and N is the total number of atoms in the crystal.

One wishes to determine the Green's functions

$$\begin{aligned} G_{kk'}(\omega) &= \tfrac{1}{2}\langle\langle C_{k'\mu}\,;\, C^\dagger_{k\mu}\rangle\rangle_\omega \ , \\ \Gamma_{kk'}(\omega) &= \tfrac{1}{2}\langle\langle \vec{\sigma}_{\mu\mu'}\cdot\vec{S}\, C_{k'\mu'}\,;\, C^\dagger_{k\mu}\rangle\rangle_\omega \ , \end{aligned} \tag{2}$$

where $\langle\langle A;\ B\rangle\rangle_\omega$ denotes the Fourier transform of the time-dependent Green's function in the notation of Zubarev.[4] $\langle\langle A;\ B\rangle\rangle_\omega$ satisfies the equation of motion

$$\omega\langle\langle A;\ B\rangle\rangle_\omega = (1/2\pi)\langle [A,\ B]_+\rangle + \langle\langle [A,H];\ B\rangle\rangle_\omega$$

or

$$\omega\langle\langle A;\ B\rangle\rangle_\omega = (1/2\pi)\langle [A,\ B]_+\rangle + \langle\langle A;\ [H,B]\rangle\rangle_\omega \ , \tag{3}$$

and the thermal average $\langle BA\rangle$ is obtained from the relation

$$\langle BA\rangle = \mathfrak{F}_\omega\{\langle\langle A;\ B\rangle\rangle_\omega\} \equiv i\lim_{\delta\to 0^+}\int_{-\infty}^{+\infty} d\omega f(\omega) \times[\langle\langle A;\ B\rangle\rangle_{\omega+i\delta} - \langle\langle A;\ B\rangle\rangle_{\omega-i\delta}] \ , \tag{4}$$

where $f(\omega)$ is the Fermi function.

The equations of motion for $G_{kk'}(\omega)$ and $\Gamma_{kk'}(\omega)$ obviously do not form a closed set. In the Nagaoka theory one terminates the hierarchy of equations of motion by means of the approximation

$$\begin{aligned} &\langle\langle (\vec{\sigma}_{\mu\mu'}\circ i\vec{\sigma}_{\nu\nu'}\times\vec{S})\, C^\dagger_{l\nu} C_{l'\nu'},\ C_{k'\mu'}\,;\, C^\dagger_{k\mu}\rangle\rangle_\omega \\ &\simeq 2\langle C^\dagger_{l\mu} C_{k'\mu}\rangle\,\Gamma_{kl'}(\omega) - 2\langle(\vec{\sigma}_{\mu\mu'}\cdot\vec{S})\, C^\dagger_{l\mu} C_{k'\mu'}\rangle\, G_{kl'}(\omega) \ . \end{aligned} \tag{5}$$

This decoupling procedure yields the "Nagaoka equations"

$$\begin{pmatrix} G_{kk'}(\omega) \\ \Gamma_{kk'}(\omega)\end{pmatrix} = \frac{1}{2\pi}\begin{pmatrix}\delta_{kk'}\\ 0\end{pmatrix} + \sum_l \begin{pmatrix} \epsilon_{k'}\,\delta_{k'l} & -J/2N \\ (J/2N)[m_{k'} - S(S+1)] & \epsilon_{k'}\,\delta_{k'l} - (J/N)(n_{k'} - \tfrac{1}{2})\end{pmatrix} \times \begin{pmatrix} G_{kl}(\omega)\\ \Gamma_{kl}(\omega)\end{pmatrix} \ , \tag{6}$$

where

$$\begin{aligned} n_{kk'} &\equiv \tfrac{1}{2}\langle C^\dagger_{k\mu} C_{k'\mu}\rangle = \mathfrak{F}_\omega\{G_{k'k}(\omega)\} \ , \\ m_{kk'} &\equiv \langle\vec{\sigma}_{\mu\mu'}\cdot\vec{S}\, C^\dagger_{k\mu} C_{k'\mu'}\rangle = 2\mathfrak{F}_\omega\{\Gamma_{k'k}(\omega)\} \ , \\ n_k &\equiv \sum_{k'} n_{k'k}, \quad m_k \equiv \sum_{k'} m_{k'k} \ . \end{aligned} \tag{7}$$

The decoupling approximation (5) attempts to take into account the correlation between the spin of the impurity and the spins of the conduction electrons which is important at low temperatures. The approximation replaces various operators by their thermal averages. Although the procedure seems somewhat arbitrary, Nagaoka[2] has demonstrated that it reproduces the most divergent logarithmic terms in each order of J when compared to perturbation theory.

The one-electron t matrix in the non-spin-flip channel defined by

$$G_{kk'}(\omega) = \frac{1}{2\pi}\left(\frac{\delta_{kk'}}{\omega-\epsilon_k} + \frac{t(\omega)}{(\omega-\epsilon_k)(\omega-\epsilon_{k'})}\right) \tag{8}$$

satisfies in the Nagaoka theory the integral equation

$$t(\omega)=\frac{-(J^2/4N)\Gamma(\omega)}{1+JG(\omega)+\frac{1}{4}J^2F(\omega)\Gamma(\omega)}\ , \tag{9}$$

where

$$F(\omega)=\frac{1}{N}\sum_k \frac{1}{\omega-\epsilon_k}\ ,$$
$$G(\omega)=\frac{1}{N}\sum_k \frac{n_k-\frac{1}{2}}{\omega-\epsilon_k}\ , \tag{10}$$
$$\Gamma(\omega)=\frac{1}{N}\sum_k \frac{m_k-S(S+1)}{\omega-\epsilon_k}\ .$$

$G(\omega)$ and $\Gamma(\omega)$ are functionals of $t(\omega)$ through n_k and m_k, respectively.

The physical content of the Nagaoka theory is now known. Hamann[5] showed that Eq. (9) could be reduced to a single integral equation for the t matrix. Zittartz and Müller-Hartmann[6] have given an exact analytic solution for $t(\omega)$ for the choice of a Lorentzian density of states symmetric about the Fermi level. These results will not be reviewed.

III. DECOUPLING PROCEDURE OF ROTH

Roth[3] has proposed a prescription for decoupling the hierarchy of equations of motion for Green's functions. In the Roth procedure the infinite set of equations of motion for retarded (advanced) Green's functions is truncated in a systematic manner once one has chosen a restricted set of operators $\{A_n\}$. For this set one approximates $[A_n, H]$, where H is the Hamiltonian, by

$$[A_n, H]\simeq \sum_m K_{nm}\, A_m\ . \tag{11}$$

The matrix K, whose elements are c numbers, is the solution of the equation

$$E=KN\ , \tag{12}$$

where the Hermitian energy and renormalization matrices are defined as

$$E_{nm}=\langle[[A_n,H],A_m^\dagger]_+\rangle,\quad N_{nm}=\langle[A_n,A_m^\dagger]_+\rangle\ . \tag{13}$$

Provided N is nonsingular, the matrix K can be determined. Substituting Eq. (11) into the equation of motion for the Green's function $\langle\langle A_n, B\rangle\rangle_\omega$ (B arbitrary), one obtains an approximate closed set of equations:

$$\omega\langle\langle A_n; B\rangle\rangle_\omega\simeq\frac{1}{2\pi}\langle[A_n, B]_+\rangle+\sum_m K_{nm}\langle\langle A_m; B\rangle\rangle_\omega\ . \tag{14}$$

The formal solution is

$$\langle\langle A_n; B\rangle\rangle_\omega\simeq\frac{1}{2\pi}\sum_m[(\omega-K)^{-1}]_{nm}\langle[A_m,B]_+\rangle\ . \tag{15}$$

For the application of this procedure to the Kondo model, we take as our basis set of operators the same set as used by Nagaoka:

$$A_{1k}=C_{k\mu},\quad A_{2k}=\vec{\sigma}_{\mu\mu'}\cdot\vec{S}C_{k\mu'}\ . \tag{16}$$

It is a straightforward task to evaluate the E and N matrices. One obtains

$$N_{kk'}=\begin{pmatrix}\delta_{kk'} & 0\\ 0 & S(S+1)\delta_{kk'}-m_{k'k}\end{pmatrix}\ , \tag{17}$$

$$E_{kk'}=\begin{pmatrix}\epsilon_k\delta_{kk'} & (J/2N)[m_{k'}^*-S(S+1)]\\ (J/2N)[m_k-S(S+1)] & E_{22,kk'}\end{pmatrix}\ , \tag{18}$$

where

$$E_{22,kk'}=\epsilon_k[S(S+1)\,\delta_{kk'}-m_{k'k}]-(J/2N)\{[m_{k'}^*-S(S+1)]+2S(S+1)\,n_k-\delta_{kk'}\textstyle\sum_l m_l+L_{kk'}\}\ , \tag{19}$$

and where $L_{kk'}$ is the following sum of thermal averages involving four conduction-electron operators and one spin operator:

$$L_{kk'}=\sum_{ll'}\{\langle\vec{\sigma}_{\nu\nu'}\cdot\vec{S}\,C_{k'\mu}^\dagger C_{l\nu}^\dagger C_{l'\nu'}C_{k\mu}\rangle-\tfrac{1}{2}\langle\vec{\sigma}_{\mu\mu'}\cdot(i\vec{\sigma}_{\nu\nu'}\times\vec{S})\,C_{k'\mu}^\dagger C_{l\nu}^\dagger C_{l'\nu'}C_{k\mu'}\rangle\}\ . \tag{20}$$

By inspection we can write the matrix K as

$$K_{kk'}=\begin{pmatrix}\epsilon_k\,\delta_{kk'} & -J/2N\\ (J/2N)[m_k-S(S+1)] & \epsilon_k\,\delta_{kk'}-(J/N)(n_k+\Delta n_{kk'}-\frac{1}{2})\end{pmatrix}\ , \tag{21}$$

where $\Delta n_{kk'}$ satisfies the equation

$$\Delta n_{kk'}=\frac{1}{2S(S+1)}\left(L_{kk'}-\delta_{kk'}\sum_l m_l+2n_k m_{k'}^*\right)+\frac{1}{S(S+1)}\sum_l m_{k'l}\,\Delta n_{kl}\ . \tag{22}$$

Comparing Eq. (21) with Eq. (6), we see that the Nagaoka approximation corresponds to $\Delta n_{kk'}=0$. Hence $\Delta n_{kk'}$ is the correction to the Nagaoka approximation required by the Roth prescription for truncating the equations of motion.

It should be noticed that Eq. (22) is an integral equation for $\Delta n_{kk'}$, where the kernel $m_{k'l}$ must be found self-consistently in terms of the eventual solution. This difficulty, however, does not pre-

vent one from carrying out the Roth prescription. In Sec. IV we show how it is possible to construct the required Green's functions.

IV. EVALUATION OF GREEN'S FUNCTIONS

Since the Green's functions are to be evaluated according to Eq. (15), one wants an explicit expression for the matrix $(\omega - K)^{-1}$. First note that $(\omega - K)^{-1} = N(\omega N - E)^{-1}$. We now attempt to find the inverse of $\omega N - E$, which we know explicitly from Eqs. (17) and (18):

$$(\omega N - E)_{kk'} = \begin{pmatrix} (\omega - \epsilon_k)\delta_{kk'} & (J/2N)[S(S+1) - m^*_{k'}] \\ (J/2N)[S(S+1) - m_k] & (\omega - \epsilon_k)[S(S+1)\delta_{kk'} - m_{k'k}] + \Delta_{kk'} \end{pmatrix} , \tag{23}$$

where

$$\Delta_{kk'} = \frac{J}{N}\,(n_k - \tfrac{1}{2})[S(S+1) - m^*_{k'}] + \frac{J}{2N}\left(L_{kk'} + 2n_k m^*_{k'} - \delta_{kk'}\sum_l m_l\right) . \tag{24}$$

Let

$$(\omega N - E)^{-1}_{k'l} \equiv \begin{pmatrix} A_{k'l}(\omega) & C_{k'l}(\omega) \\ B_{k'l}(\omega) & D_{k'l}(\omega) \end{pmatrix} . \tag{25}$$

The matrices A, B, C, and D are determined by the equations

$$(\omega - \epsilon_k)A_{kl}(\omega) + \frac{J}{2N}\sum_{k'}\,[S(S+1) - m^*_{k'}]\,B_{k'l}(\omega) = \delta_{kl} , \tag{26}$$

$$\frac{J}{2N}\,[S(S+1) - m_k]\sum_{k'} A_{k'l}(\omega) + (\omega - \epsilon_k)\sum_{k'}\,[S(S+1)\delta_{kk'} - m_{k'k}]\,B_{k'l}(\omega) + \frac{J}{N}\,(n_k - \tfrac{1}{2})\sum_{k'}\,[S(S+1) - m^*_{k'}]\,B_{k'l}(\omega) + \frac{J}{2N}\sum_{k'}\left(L_{kk'} + 2n_k m^*_{k'} - \delta_{kk'}\sum_l m_l\right)B_{k'l}(\omega) = 0 , \tag{27}$$

$$(\omega - \epsilon_k)\,C_{kl}(\omega) + \frac{J}{2N}\sum_{k'}\,[S(S+1) - m^*_{k'}]\,D_{k'l}(\omega) = 0 , \tag{28}$$

$$\frac{J}{2N}\,[S(S+1) - m_k]\sum_{k'} C_{k'l}(\omega) + (\omega - \epsilon_k)\sum_{k'}\,[S(S+1) - m_{k'k}]\,D_{k'l}(\omega) + \sum_{k'}\,\Delta_{kk'}D_{k'l}(\omega) = \delta_{kl} . \tag{29}$$

Since N and E are Hermitian matrices,

$$A^*_{kk'}(\omega) = A_{k'k}(\omega^*) , \tag{30}$$

$$D^*_{kk'}(\omega) = D_{k'k}(\omega^*) , \tag{31}$$

$$B^*_{kk'}(\omega) = C_{k'k}(\omega^*) . \tag{32}$$

It is clear from Eq. (28) that $C_{kl}(\omega)$ is of the form

$$C_{kl}(\omega) = g_l(\omega)/(\omega - \epsilon_k) . \tag{33}$$

Using Eq. (32), we may rewrite Eq. (26) as

$$(\omega - \epsilon_k)A_{kl}(\omega) + \frac{J}{2N}\,\frac{1}{\omega - \epsilon_l} \times \sum_{k'}\,[S(S+1) - m^*_{k'}]\,g^*_{k'}(\omega^*) = \delta_{kl} . \tag{34}$$

Hence,

$$A_{kl}(\omega) = \frac{\delta_{kl}}{\omega - \epsilon_k} + \frac{t(\omega)}{(\omega - \epsilon_k)(\omega - \epsilon_l)} , \tag{35}$$

where

$$t(\omega) = \frac{J}{2N}\sum_k\,[m^*_k - S(S+1)]\,g^*_k(\omega^*) = t^*(\omega^*) , \tag{36}$$

where the last equality follows from Eq. (30). The set of functions $g_k(\omega)$ are determined by Eq. (27), which we rewrite as

$$(\omega - \epsilon_k)\sum_{k'}\,[S(S+1) - m_{k'k}]\,g^*_{k'}(\omega^*) + \frac{J}{2N}\,[S(S+1) - m_k] \times [1 + NF(\omega)t(\omega)] - 2(n_k - \tfrac{1}{2})t(\omega) + \frac{J}{2N}\sum_{k'}\left(L_{kk'} + 2n_k m^*_{k'} - \delta_{kk'}\sum_l m_l\right)g^*_{k'}(\omega^*) = 0 , \tag{37}$$

where $F(\omega)$ is given by definition (10).

All the required Green's functions can be evaluated by using only the 11, 12, and 21 elements of $(\omega - K)^{-1}$. Recalling that $(\omega - K)^{-1} = N(\omega N - E)^{-1}$, we use Eqs. (17), (32), (33), and (35) to obtain

$$(\omega - K)^{-1}_{11,kk'} = \frac{\delta_{kk'}}{\omega - \epsilon_k} + \frac{t(\omega)}{(\omega - \epsilon_k)(\omega - \epsilon_{k'})} , \tag{38}$$

$$(\omega - K)^{-1}_{12,kk'} = \frac{g_{k'}(\omega)}{\omega - \epsilon_k} , \tag{39}$$

$$(\omega - K)^{-1}_{21,kk'} = \sum_l\,[S(S+1)\,\delta_{kl} - m_{lk}]\,\frac{g^*_l(\omega^*)}{\omega - \epsilon_{k'}} . \tag{40}$$

The thermal averages appearing in Eq. (37), which determines a self-consistent set of functions $g_k(\omega)$, are evaluated by use of Eq. (4). One readily obtains

$$n_{kk'} = \frac{1}{2\pi}\,\mathfrak{F}_\omega\left\{\frac{\delta_{kk'}}{\omega-\epsilon_k} + \frac{t(\omega)}{(\omega-\epsilon_k)(\omega-\epsilon_k')}\right\}, \quad (41)$$

$$m_{kk'} = \frac{1}{\pi}\,\mathfrak{F}_\omega\left\{\sum_l [S(S+1)\,\delta_{kl} - m_{lk}]\frac{g_l^*(\omega)}{\omega-\epsilon_{k'}}\right\}. \quad (42)$$

In order to complete the equations it would appear that one must also evaluate $L_{kk'}$. However, $L_{kk'}$ is a sum of thermal averages which are not of the form $\langle A_n^\dagger A_m\rangle$, where A_n and A_m are numbers of our basis set of operators. This leads to some arbitrariness in the evaluation of $L_{kk'}$. Instead of directly evaluating $L_{kk'}$, we shall show that $g_l(\omega)$ can be determined by requiring a certain exact relationship between the Green's functions to be satisfied by the approximate Green's functions. First we demonstrate certain results.

The function $t(\omega)$ is clearly the one-electron t matrix. The thermal averages $n_{k'}$ and $m_{k'}$ are obtained from Eqs. (41) and (42) by summing over the index k:

$$n_{k'} = \frac{1}{2\pi}\,\mathfrak{F}_\omega\left\{\frac{1+NF(\omega)t(\omega)}{\omega-\epsilon_{k'}}\right\}, \quad (43)$$

$$m_{k'} = -\frac{2N}{\pi J}\,\mathfrak{F}_\omega\left\{\frac{t(\omega)}{\omega-\epsilon_{k'}}\right\}. \quad (44)$$

It is clear from Eq. (44) that m_k is real since $t^*(\omega) = t(\omega^*)$. Then it immediately follows that

$$g_k^*(\omega) = g_k(\omega^*) \quad (45)$$

and

$$m_{kk'} = m_{k'k}. \quad (46)$$

We now proceed to evaluate $g_k(\omega)$. First we note that if one uses the second form for the equation of motion given in Eq. (3), one immediately obtains the exact equation

$$(\omega-\epsilon_{k'})\langle\langle\vec{\sigma}_{\mu\mu'}\cdot\vec{S}C_{k\mu'};C^\dagger_{k'\mu}\rangle\rangle_\omega = -\frac{J}{2N}\sum_l\langle\langle\vec{\sigma}_{\mu\mu'}\circ\vec{S}C_{k\mu'};\vec{\sigma}_{\mu'',\mu}\circ\vec{S}C^\dagger_{l\mu'',}\rangle\rangle_\omega. \quad (47)$$

Consequently,

$$\mathfrak{F}_\omega\{(\omega-\epsilon_{k'})\langle\langle\vec{\sigma}_{\mu\mu'}\cdot\vec{S}C_{k\mu'};C^\dagger_{k'\mu}\rangle\rangle_\omega\} = -\frac{J}{2N}\sum_l\langle(\vec{\sigma}\cdot\vec{S})^2_{\mu'',\mu'}C^\dagger_{l\mu'',}C_{k\mu'}\rangle = \frac{J}{2N}[m_k - 2S(S+1)n_k]. \quad (48)$$

This is an exact result. If one now evaluates

$$(\omega-\epsilon_{k'})\langle\langle\vec{\sigma}_{\mu\mu'}\cdot\vec{S}C_{k\mu'};C^\dagger_{k'\mu}\rangle\rangle_\omega$$

by means of the Roth prescription, the following relationship is obtained:

$$\frac{1}{2\pi}\,\mathfrak{F}_\omega\left\{\sum_l S(S+1)\delta_{kl} - m_{lk}\,g_l(\omega)\right\} = \frac{J}{4N}[m_k - 2S(S+1)n_k]. \quad (49)$$

We shall require that $g_k(\omega)$ be consistent with this relation. It should be noted that Eq. (47) could have been obtained from Eq. (28), which demonstrates that the Roth prescription is consistent with this exact result.

Now consider Eq. (37). By dividing by $\omega-\epsilon_p$ and performing the $\mathfrak{F}_\omega$ operation, we obtain

$$\mathfrak{F}_\omega\left\{\sum_l [S(S+1)-m_{lk}]g_l(\omega)\left(1+\frac{\epsilon_p-\epsilon_k}{\omega-\epsilon_p}\right)\right\} + \frac{J}{2N}[S(S+1)-m_k]\,\mathfrak{F}_\omega\left\{\frac{1+NF(\omega)t(\omega)}{\omega-\epsilon_p}\right\} - 2(n_k-\tfrac{1}{2})\,\mathfrak{F}_\omega\left\{\frac{t(\omega)}{\omega-\epsilon_p}\right\} + \frac{J}{2N}\,\mathfrak{F}_\omega\left\{\sum_l\left(L_{kl}+2n_km_l-\delta_{kl}\sum_q m_q\right)\frac{g_l(\omega)}{\omega-\epsilon_p}\right\} = 0. \quad (50)$$

Using Eqs. (42)–(44), together with the relationship (49), we find

$$\frac{1}{2\pi}\,\frac{J}{N}\,\mathfrak{F}_\omega\left\{\sum_l\left(L_{kl}+2n_km_l-\delta_{kl}\sum_q m_q\right)\frac{g_l(\omega)}{\omega-\epsilon_p}\right\} = (\epsilon_k-\epsilon_p)m_{kp} - (J/N)\{(n_k-\tfrac{1}{2})[m_p-S(S+1)] - [m_k-S(S+1)](n_p-\tfrac{1}{2})\}. \quad (51)$$

Equation (51) should be viewed as a condition on L_{kl} resulting from requiring the exact result, Eq. (47), be satisfied by the approximate Green's functions. We shall now show that one can evaluate $g_k(\omega)$ with the aid of Eq. (51).

An equivalent equation to Eq. (37) for determining the functions $g_k(\omega)$ can be obtained from Eqs. (23) and (25) by treating $(\omega N - E)^{-1}$ as the left inverse. One readily obtains

$$[1+NF(\omega)t(\omega)]\,\frac{J}{2N}[S(S+1)-m_k] + \sum_l g_l(\omega)(\omega-\epsilon_l)[S(S+1)\delta_{lk}-m_{kl}] + \frac{J}{N}\sum_l g_l(\omega)(n_l-\tfrac{1}{2})[S(S+1)-m_k] + \frac{J}{2N}\sum_l g_l(\omega)\left(L_{lk}+2n_lm_k-\delta_{lk}\sum_q m_q\right) = 0. \quad (52)$$

We now multiply this equation by $g_k(\omega')/(\omega'-\epsilon_p)$ sum over the index k, and operate with $\mathfrak{F}_{\omega'}$. This

yields

$$-[1+NF(\omega)t(\omega)]\,\mathfrak{F}_{\omega'}\left\{\frac{t(\omega')}{\omega'-\epsilon_p}\right\}$$
$$+\sum_l g_l(\omega)(\omega-\epsilon_l)\,\mathfrak{F}_{\omega'}\left\{\sum_k [S(S+1)\,\delta_{lk} - m_{kl}]\,\frac{g_k(\omega')}{\omega'-\epsilon_p}\right\} - 2\sum_l g_l(\omega)(n_l-\tfrac{1}{2})\,\mathfrak{F}_{\omega'}\left\{\frac{t(\omega')}{\omega'-\epsilon_p}\right\}$$
$$+\frac{J}{2N}\sum_l g_l(\omega)\,\mathfrak{F}_{\omega'}\left\{\sum_k\left(L_{lk}+2n_l m_k - \delta_{lk}\sum_q m_q\right)\frac{g_k(\omega')}{\omega'-\epsilon_p}\right\}=0\,. \tag{53}$$

Equation (53) may be rewritten with the aid of Eqs. (42), (44), and (51) as

$$[1+NF(\omega)t(\omega)]m_p+\frac{2N}{J}\sum_l g_l(\omega)(\omega-\epsilon_l)\,m_{lp}$$
$$+2\sum_l g_l(\omega)(n_l-\tfrac{1}{2})m_p$$
$$+\frac{2N}{J}\sum_l g_l(\omega)\left((\epsilon_l-\epsilon_p)\,m_{lp}-\frac{J}{N}\{(n_l-\tfrac{1}{2})[m_p-S(S+1)]\right.$$
$$\left.-[m_l-S(S+1)](n_p-\tfrac{1}{2})\}\right)=0\,. \tag{54}$$

This is a convenient form since this equation does not involve the higher-order correlation functions $L_{kk'}$. Equations (54), (41), and (42) are a complete set of equations to be solved self-consistently.

The self-consistent solution is

$$g_k(\omega)=\frac{-J/2N}{\omega-\epsilon_k}\,\frac{1+NF(\omega)t(\omega)}{1+JG(\omega)}\,, \tag{55}$$

with

$$t(\omega)\equiv\frac{J}{2N}\sum_k[m_k-S(S+1)]\,g_k(\omega)$$
$$=\frac{-(J^2/4N)\,\Gamma(\omega)}{1+JG(\omega)+\frac{1}{4}J^2F(\omega)\Gamma(\omega)}\,, \tag{56}$$

where $G(\omega)$ and $\Gamma(\omega)$ are defined by Eq. (10). That $g_k(\omega)$, as given by Eq. (55), is a solution becomes immediately obvious once one demonstrates that

$$(\epsilon_l-\epsilon_p)\,m_{lp}=(J/N)\{(n_l-\tfrac{1}{2})[m_p-S(S+1)]$$
$$-[m_l-S(S+1)](n_p-\tfrac{1}{2})\} \tag{57}$$

is consistent with Eqs. (55) and (42). The demonstration is straightforward.

V. DISCUSSION OF RESULTS

The result for $t(\omega)$ given by Eq. (56) is identical to the t matrix in the Nagaoka theory. This suggests that the decoupling is the same in the Roth scheme as in the Nagaoka approximation. Recall that the correction to the Nagaoka decoupling required by the Roth prescription was given by $\Delta n_{kk'}$, which satisfied Eq. (22). It is clear from Eq. (22) that $\Delta n_{kk'}$ is zero if

$$L_{kk'}=\delta_{kk'}\textstyle\sum_l m_l-2n_k m_{k'}\,. \tag{58}$$

This relation can be shown to be consistent with $g_k(\omega)$ given by Eq. (55) by substituting for $g_k(\omega)$ in Eq. (37). One immediately obtains

$$\sum_{k'}\left(L_{kk'}-\delta_{kk'}\sum_l m_l+2n_k m_{k'}\right)\times\frac{1+NF(\omega)t(\omega)}{1+JG(\omega)}\,\frac{1}{\omega-\epsilon_{k'}}=0\,. \tag{59}$$

Since ω is arbitrary, this implies Eq. (58). Therefore, we conclude that the decoupling is the same for our application of the Roth scheme.

It is interesting to note that Eq. (58) can *not* be obtained directly from the definition of $L_{kk'}$, given by Eq. (20), using a straightforward generalization of the Nagaoka approximation. If the Nagaoka approximation, Eq. (5), is used to approximate the appropriate Green's function required to determine the second term in expression (20) for $L_{kk'}$, one immediately obtains

$$\sum_{ll'}\langle\vec{\sigma}_{\mu\mu'}\cdot(i\vec{\sigma}_{\nu\nu'}\times\vec{S})C^\dagger_{k'\mu}C^\dagger_{l\nu}C_{l'\nu'}C_{k\mu'}\rangle \simeq 2n_k m_{k'}-2m_k m_{k'}\,. \tag{60}$$

In order to evaluate the first term we introduce an approximation similar to Eq. (5) and obtain

$$\sum_{ll'}\langle\vec{\sigma}_{\nu\nu'}\cdot\vec{S}C^\dagger_{k'\mu}C^\dagger_{l\nu}C_{l'\nu'}C_{k\mu}\rangle \simeq 2n_{k'k}\sum_l m_l-n_{k'}m_k-n_k m_{k'}\,. \tag{61}$$

Equation (61) contains all the nonvanishing terms resulting from replacing combinations of operators by their average values. Hence the straightforward generalization of the Nagaoka approximation is

$$L_{kk'}\simeq 2n_{kk'}\textstyle\sum_l m_l-2n_k m_{k'}\,. \tag{62}$$

Note that this result is inconsistent with the determination of $L_{kk'}$ based on the Roth prescription.

Rather than assume that the averages in $L_{kk'}$ factor according to a Nagaoka approximation, we can make use of Eq. (15) of the Roth-approximation scheme to evaluate the appropriate Green's functions for a direct evaluation of $L_{kk'}$. Note that the operator B in Eq. (15) is arbitrary according to the formulation of the Roth scheme. If we choose

$$B_{k'\mu'}=\sum_{ll'}\{\vec{\sigma}_{\nu\nu'}\cdot\vec{S}C^\dagger_{k'\mu'}C^\dagger_{l\nu}C_{l'\nu'} - \tfrac{1}{2}\vec{\sigma}_{\mu\mu'}\cdot(i\vec{\sigma}_{\nu\nu'}\times\vec{S})C^\dagger_{k'\mu}C_{l\nu}C_{l'\nu'}\}, \tag{63}$$

then $L_{kk'}$ can be evaluated from the Green's function $\langle\langle C_{k\mu'};\ B_{k'\mu'}\rangle\rangle_\omega$. Using Eq. (15), we find

$$L_{kk'} \simeq 2n_{kk'} \sum_l m_l - 2n_k m_{k'} + \frac{1}{2\pi} \mathfrak{F}_\omega \left\{ \sum_l \frac{g_l(\omega)}{\omega - \epsilon_k} \left(L_{lk'} + m_{k'} - \delta_{lk'} \sum_p m_p \right) \right\} . \quad (64)$$

However, this result is also inconsistent with Eq. (58). The lack of consistency illustrates a basic difficulty associated with the Roth scheme. If we had used Eq. (64) to substitute for $L_{kk'}$ in Eq. (37), the resulting t matrix would undoubtably be different from the Nagaoka result. The result would no longer reproduce the logarithmic terms of the perturbation theory. A calculation using Eq. (64) has not been carried out because of the formidable mathematical difficulties involved in determining $g_k(\omega)$ from Eq. (37).[7]

The procedure whereby $L_{kk'}$ is determined by requiring the approximate Green's functions to be consistent with the exact relationship expressed in Eq. (47) is certainly the preferable procedure. This produces a completely self-consistent application of the Roth scheme for determining the t matrix. One should not, however, conclude that Eq. (58) gives a valid approximation for $L_{kk'}$. The basis set of operators is inadequate to describe such higher-order averages. This shows itself in the lack of agreement between Eqs. (58), (62), and (64). Difficulties must necessarily arise in applying the Roth procedure if one is unable to avoid evaluating such higher-order averages.

Our treatment yields increased confidence in the t matrix of the Nagaoka theory. The t matrix determines the resistivity, specific heat, and electron-spin–impurity-spin correlation function. The results for these quantities seem to be qualitatively correct. Also, an attempt has been made to determine the magnetic susceptibility within the Nagaoka theory.[2,5] The result is an infinite $T = 0$ susceptibility, which is unreasonable. However, it should be noticed that the calculation of the susceptibility requires the evaluation of $\langle \vec{S}^2_{\rm tot} \rangle$, where

$$\vec{S}_{\rm tot} = \vec{S} + \tfrac{1}{2} \sum_k \vec{\sigma}_{\mu\mu'} C^\dagger_{k\mu} C_{k\mu'} .$$

Our results indicate that such higher-order averages are not evaluated accurately by a generalization of the Nagaoka approximation. Therefore, it is not surprising that one obtains unreasonable results for the susceptibility. Also, if one is to use the Roth scheme to calculate the susceptibility, the basis set of operators must be enlarged.

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