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Reformulation of the Nagaoka Equations*

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The Green's-function equations describing an electron gas in the presence of a magnetic impurity have been approximated by Nagaoka by means of a truncation procedure that keeps correlations between the spins of the impurity and a conduction electron, but neglects higher correlations. Nagaoka's approximate equations are examined here and reformulated as a one-dimensional nonlinear equation. This equation is solved for temperatures not too close to T_K, a characteristic temperature of the system, and shown to have two solutions: a normal solution which exists at all temperatures and a condensed solution valid only below T_K. Perturbative corrections to the normal solution are presented.

SINCE Kondo's[1] demonstration that the transition probability of conduction electrons in the presence of a magnetic impurity exhibits a logarithmic divergence at zero temperature, there have been a number of attempts to treat such a system by nonperturbative techniques.[2] Although there appears to be some relationship between two of these methods,[3] there remain differences, and there is as yet no compelling reason to favor one approach over another. Each approach has its advocates.

It seems useful, therefore, to examine the various theories more closely to see what, indeed, they actually predict. It is the purpose of this paper to present one of these theories, that of Nagaoka,[2] in a somewhat different mathematical framework that explicitly exhibits the approximations within the theory used by Nagaoka, and that may suggest alternative approximations.

The starting point for all of these theories is the s-d interaction Hamiltonian

$$H=\sum_{\mathbf{k},\alpha}\xi_{\mathbf{k}}C^{\dagger}{}_{\mathbf{k}\alpha}C_{\mathbf{k}\alpha}-\frac{J}{2N}\sum_{\mathbf{k},\mathbf{k}',\alpha,\beta}C^{\dagger}{}_{\mathbf{k}\alpha}C_{\mathbf{k}'\beta}\boldsymbol{\sigma}_{\alpha\beta}\cdot\mathbf{S}. \quad (1)$$

Here $C^{\dagger}{}_{\mathbf{k}\alpha}$ creates a conduction electron of momentum $\mathbf{k}$ and spin α, ξ_k is the conduction-electron energy measured from the Fermi energy, $\mathbf{S}$ is the spin operator for the impurity moment (which we take to have spin $\frac{1}{2}$), N is the number of electrons, and J is the strength of the exchange interaction, taken here to be a contact interaction. (This will require later that certain integrals will have to be cut off.) This Hamiltonian has been shown to follow, under suitable conditions, from the Anderson Hamiltonian[4] by Schrieffer and Wolff.[5]

Nagaoka writes the equations of motion for the retarded Green's functions

$$G_{\mathbf{k}\mathbf{k}'}(\omega)=\langle C_{\mathbf{k}'\uparrow}|C^{\dagger}{}_{\mathbf{k}\uparrow}\rangle \quad (2)$$

and

$$\Gamma_{\mathbf{k}\mathbf{k}'}(\omega)=\langle C_{\mathbf{k}'\uparrow}S_z+C_{\mathbf{k}'\downarrow}S_-|C^{\dagger}{}_{\mathbf{k}\uparrow}\rangle. \quad (3)$$

He then introduces his decoupling scheme, factoring higher-order Green's functions by replacing certain products of operators by their expectation values. His

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[1] J. Kondo, Progr. Theoret. Phys. (Kyoto) **32**, 37 (1964).
[2] Y. Nagaoka, Phys. Rev. **138**, A1112 (1965); A. A. Abrikosov, Physics **2**, 5 (1965); H. Suhl, Phys. Rev. **138**, A515 (1965).
[3] S. D. Silverstein and C. B. Duke, in Twelfth Annual Conference on Magnetism and Magnetic Materials (to be published).
[4] P. W. Anderson, Phys. Rev. **124**, 41 (1961).
[5] J. R. Schrieffer and P. A. Wolff, Phys. Rev. **149**, 491 (1966).

approximation may be written as

$$\sum_{\beta,\gamma,\delta}\langle C^\dagger{}_{p\gamma}C_{q\delta}C_{1\beta}(\boldsymbol{\sigma}_{\gamma\delta}\times\mathbf{S})\cdot\boldsymbol{\sigma}_{\alpha\beta}|C^\dagger{}_{k\alpha}\rangle \approx -2i\langle C^\dagger{}_{p\gamma}C_{1\alpha}\rangle\sum_\beta\langle\mathbf{S}\cdot\boldsymbol{\sigma}_{\alpha\beta}C_{q\beta}|C^\dagger{}_{k\alpha}\rangle + i[\sum_{\beta\gamma}\langle C^\dagger{}_{p\gamma}\mathbf{S}\cdot\boldsymbol{\sigma}_{\gamma\beta}C_{1\beta}\rangle]\langle C_{q\alpha}|C^\dagger{}_{k\alpha}\rangle. \quad (4)$$

The resulting equations of motion are then "solved," for the case $\langle S_z\rangle=0$, to yield the results [Eqs. (2.15) through (2.21) of Nagaoka[2]]

$$2\pi G_{kk'}(\omega)=\frac{\delta_{k,k'}}{\omega-\xi_k}-\frac{J}{4N}\frac{1}{(\omega-\xi_k)(\omega-\xi_{k'})}\gamma(\omega), \quad (5)$$

$$2\pi\Gamma_{kk'}(\omega)=\frac{J}{2N}\frac{1}{(\omega-\xi_k)(\omega-\xi_{k'})}[(m_{k'}-\tfrac{3}{4})g(\omega)-(n_{k'}-\tfrac{1}{2})\gamma(\omega)], \quad (6)$$

where

$$\gamma(\omega)=\frac{J\Gamma(\omega)}{1+JG(\omega)+\frac{1}{4}J^2F(\omega)\Gamma(\omega)}, \quad (7)$$

$$g(\omega)=\frac{1+JG(\omega)}{1+JG(\omega)+\frac{1}{4}J^2F(\omega)\Gamma(\omega)}=1-\tfrac{1}{4}JF(\omega)\gamma(\omega), \quad (8)$$

with

$$F(\omega)=\frac{1}{N}\sum_k\frac{1}{\omega-\xi_k}, \quad (9)$$

$$G(\omega)=\frac{1}{N}\sum_k\frac{n_k-\frac{1}{2}}{\omega-\xi_k}, \quad (10)$$

$$\Gamma(\omega)=\frac{1}{N}\sum_k\frac{m_k-\frac{3}{4}}{\omega-\xi_k}, \quad (11)$$

$$n_k=\sum_1\langle C^\dagger{}_{1\uparrow}C_{k\uparrow}\rangle, \quad (12)$$

$$m_k=3\sum_1\langle C^\dagger{}_{1\uparrow}C_{k\downarrow}S_-\rangle, \quad (13)$$

and, because these are retarded Green's functions, ω is to be interpreted as $\omega+i\epsilon$, where ϵ is a positive infinitesimal. This is not a solution yet because one still must solve self-consistently for the expectation values n_k and m_k.

Now,

$$n_k=-2\int_{-\infty}^{\infty}d\omega\, f(\omega)\,\mathrm{Im}G_k(\omega), \quad (14)$$

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

$$G_k(\omega)=\sum_1 G_{1k}(\omega)=\frac{1}{2\pi}\frac{1}{\omega-\xi_k+i\epsilon}g(\omega). \quad (15)$$

We note that

$$G(\omega)+\tfrac{1}{2}F(\omega)=\frac{1}{N}\sum_k\frac{n_k}{\omega-\xi_k+i\epsilon}. \quad (16)$$

We follow Nagaoka in assuming that the density of states varies slowly over the conduction band and may be replaced by ρ, its value at the Fermi surface, so that

$$\sum_k\to\rho\int d\xi_k. \quad (17)$$

Then

$$G(\omega)+\tfrac{1}{2}F(\omega)=\frac{\rho}{N}\int_{-\infty}^{\infty}d\xi\frac{1}{\omega-\xi+i\epsilon}\frac{i}{2\pi}\int_{-\infty}^{\infty}d\omega'\,f(\omega')\times\left[\frac{g(\omega'+i\epsilon)}{\omega'-\xi+i\epsilon}-\frac{g(\omega'-i\epsilon)}{\omega'-\xi-i\epsilon}\right]$$

$$=\frac{\rho}{N}\int_{-\infty}^{\infty}d\xi\frac{f(\xi)}{\omega-\xi+i\epsilon}g(\xi-i\epsilon). \quad (18)$$

Further, since m_k is real we have

$$m_k=m^*{}_k=3\sum_1\langle C^\dagger{}_{k\uparrow}C_{1\downarrow}S_-\rangle=-2\int_{-\infty}^{\infty}d\omega\,f(\omega)\,\mathrm{Im}\tilde{\Gamma}_k(\omega), \quad (19)$$

where

$$\tilde{\Gamma}_k(\omega)=\sum_1\Gamma_{k1}(\omega)=\frac{1}{4\pi}\frac{1}{\omega-\xi_k+i\epsilon}\gamma(\omega). \quad (20)$$

Hence

$$\Gamma(\omega)+\tfrac{3}{4}F(\omega)=\frac{1}{N}\sum_k\frac{m_k}{\omega-\xi_k+i\epsilon}=\frac{\rho}{N}\int_{-\infty}^{\infty}d\xi\frac{f(\xi)}{\omega-\xi+i\epsilon}\gamma(\xi-i\epsilon). \quad (21)$$

Now, using the approximation (17), we have

$$F(\omega\pm i\epsilon)=\frac{1}{N}\sum_k\frac{1}{\omega-\xi_k\pm i\epsilon}\approx\frac{\rho}{N}\int_{-\infty}^{\infty}\frac{d\xi}{\omega-\xi\pm i\epsilon}=\mp i\pi(\rho/N). \quad (22)$$

If we combine this with (18) and (21), noting (8), we get the relation

$$G(\omega)=G_0(\omega)-\frac{i\pi}{4}\frac{J\rho}{N}\left[\Gamma(\omega)-\frac{3i\pi}{4}\frac{\rho}{N}\right], \quad (23)$$

where

$$G_0(\omega)=\frac{1}{N}\sum_k\frac{f(\xi_k)-\frac{1}{2}}{\omega-\xi_k}=\frac{\rho}{N}\int_{-D}^{D}d\xi\frac{f(\xi)}{\omega-\xi+i\epsilon}+\frac{i\pi}{2}\frac{\rho}{N} \quad (24)$$

and we have introduced the cutoff D, following Nagaoka.

Let us define

$$g(\omega)=\omega/[\omega+A(\omega)] \tag{25}$$

and use (23) to eliminate $\Gamma(\omega)$ in (8). We then solve (8) for $JG(\omega)$ as a function of $A(\omega)$ and insert that in (18). The resulting equation[6] is [noting that $A^*(\xi+i\epsilon)=A(\xi-i\epsilon)$]

$$\left[1+\frac{i\pi}{2}\frac{J\rho}{N}+\frac{J\rho}{N}\int_{-D}^{D}d\xi\frac{f(\xi)}{\omega-\xi+i\epsilon}-\frac{3\pi^2}{16}\left(\frac{J\rho}{N}\right)^2\right]\frac{\omega}{\omega-A(\omega)}$$
$$=1+\frac{i\pi}{2}\frac{J\rho}{N}+\frac{J\rho}{N}\int_{-D}^{D}d\xi\frac{f(\xi)}{\omega-\xi+i\epsilon}\frac{\xi}{\xi+A^*(\xi)}. \tag{26}$$

This is the basic one-dimensional nonlinear equation which, with the exception of the constant density of states assumption (17), follows exactly from Nagaoka's basic approximation (4).

We wish to examine this equation in the limit

$$J\rho/N\ll 1 \quad \text{(weak coupling)}. \tag{27}$$

In this limit, one might suppose that we could neglect the term proportional to $(J\rho/N)^2$ in brackets on the left-hand side of (26). The resultant equation

$$\left[1+\frac{i\pi}{1}\frac{J\rho}{N}+\frac{J\rho}{N}\int_{-D}^{D}d\xi\frac{f(\xi)}{\omega-\xi+i\epsilon}\right]\frac{\omega}{\omega-A(\omega)}$$
$$=1+\frac{i\pi}{2}\frac{J\rho}{N}+\frac{J\rho}{N}\int_{-D}^{D}d\xi\frac{f(\xi)}{\omega-\xi+i\epsilon}\frac{\xi}{\xi+A^*(\xi)} \tag{28}$$

then is easily seen to have two solutions:

(1) normal solution:

$$A(\omega)=0. \tag{29}$$

This is a solution of (28) for all temperatures, and gives the noninteracting conduction-electron Green's function.

(2) condensed solution[7]:

$$A(\omega)=i\Delta \quad (\Delta \text{ real}), \quad (\Delta>0). \tag{30}$$

[This corresponds to a peak in $G_{kk'}(\omega)$ at $\omega=0$, of width Δ.] Here Δ is determined by

$$1=-\frac{i\pi}{2}\frac{J\rho}{N}+\frac{J\rho}{N}\int_{-D}^{D}d\xi\frac{f(\xi)}{\xi-i\Delta}$$
$$=-\frac{J\rho}{N}\int_{0}^{D}d\xi\frac{\xi}{\xi^2+\Delta^2}\tanh\frac{\xi}{2T}. \tag{31}$$

This is a solution providing $J<0$ (antiferromagnetic coupling) and $T<T_K$, where T_K is a critical temperature determined by

$$1=-\frac{J\rho}{N}\int_{0}^{D}\frac{d\xi}{\xi}\tanh\frac{\xi}{2T_K} \tag{32}$$

or

$$T_K=(2\gamma D/\pi)\exp(N/J\rho), \tag{33}$$

where $\ln\gamma=0.577\cdots$ is Euler's constant.

Now, we can calculate the conditions under which it is permissible to drop the $(J\rho/N)^2$ term in (26) to give (28). We notice that as $T\rightarrow T_K-$, and therefore $\Delta\rightarrow 0+$, (31) may be written

$$0=1+\frac{i\pi}{2}\frac{J\rho}{N}+\frac{J\rho}{N}\int_{-D}^{D}d\xi\frac{f(\xi)}{-\xi+i\epsilon}=1+JG_0(0) \quad (T=T_K). \tag{34}$$

Hence, everything in the brackets on the left-hand side of (26) vanishes except the $(J\rho/N)^2$ term at $T=T_K$ and $\omega=0$. We therefore must keep the $(J\rho/N)^2$ term in the vicinity of T_K.

More precisely, near $T=T_K$, the term in the brackets of (26) at $\omega=0$ is (taking $\Delta\ll T$) approximately

$$\frac{J\rho}{N}\frac{T_K-T}{T_K}-\frac{3\pi^2}{16}\left(\frac{J\rho}{N}\right)^2, \tag{35}$$

which, incidentally, implies that near T_K

$$\frac{\Delta}{T}\approx\frac{4}{\pi}\frac{T_K-T}{T_K}. \tag{36}$$

Hence, the $(J\rho/N)^2$ term may be dropped whenever

$$\frac{|T-T_K|}{T_K}\gg\frac{3\pi^2}{16}\frac{|J|\rho}{N}. \tag{37}$$

As long as the condition (37) is satisfied, (28) is a good approximation to (26), and the two solutions (29) and (30) are valid. Thus for $T<T_K$ there are two solutions to the Nagaoka equations. It is easy to verify that the condensed solution has a lower energy than the normal solution for $T<T_K$. Hence the Nagaoka equations seem to imply that there is, in the vicinity of T_K, some sort of phase change, where the system changes from the normal to the condensed solution.

If we consider the normal solution (29), then the first thing one might try is a perturbative expansion

[6] Since completion of this work we have discovered that D. R. Hamann has derived essentially the same equation independently (to be published).

[7] It should be noted that Suhl's theory, based on an S-matrix formulation of the problem, implies that the scattering amplitudes and transport coefficients are smooth functions of temperature across T_K [cf. H. Suhl and D. Wong, Physics (to be published)]. This does not, however, preclude a gradual change in properties in the vicinity of T_K [cf. H. Suhl, Lectures presented at the 1966 International School of Physics "Enrico Fermi," Varenna, Italy (unpublished)].

of $A(\omega)$ in powers of $J\rho$-N. The result of such an expansion is

$$A(\omega)=\frac{3\pi^2}{16}\left(\frac{J\rho}{N}\right)^2\omega\left[1-\frac{i\pi}{2}\left(\frac{J\rho}{N}\right)-2\frac{J\rho}{N}\int_{-D}^{D}d\xi\frac{f(\xi)}{\omega-\xi+i\epsilon}\right]+O\left[\left(\frac{J\rho}{N}\right)^4\right]$$

$$=\frac{3\pi^2}{16}\left(\frac{J\rho}{N}\right)^2\omega\left[1-2JG_0(\omega)+\frac{i\pi}{2}\left(\frac{J\rho}{N}\right)\right]+O\left[\left(\frac{J\rho}{N}\right)^4\right]. \quad (38)$$

This solution is presumably valid at high temperatures, and we may expect it to be valid as long as the expression in the brackets on the left-hand side of (26) does not vanish. We call this expression $H(\omega)$,

$$H(\omega)=1+\frac{J\rho}{N}\int_{-D}^{D}d\xi\frac{f(\xi)-\frac{1}{2}}{\omega-\xi+i\epsilon}-\frac{3\pi^2}{16}\left(\frac{J\rho}{N}\right)^2$$

$$=1+JG_0(\omega+i\epsilon)-\frac{3\pi^2}{16}\left(\frac{J\rho}{N}\right)^2$$

$$=1+\frac{J\rho}{N}\left[\ln\frac{D}{2\pi T}-\psi\left(\frac{1}{2}-\frac{i\omega}{2\pi T}\right)\right]-\frac{3\pi^2}{16}\left(\frac{J\rho}{N}\right)^2, \quad (39)$$

where $\psi(z)$ is the digamma function, the logarithmic derivative of the γ function. The zeros of $H(\omega)$ lie on the imaginary ω axis, and for T sufficiently large there are no zeros in the upper half-plane. However, as T is lowered, for $J<0$, one zero moves up into the upper half-plane, thus producing, we may assume, a new behavior in $A(\omega)$ and invalidating (38). The temperature at which this happens we call T_K' and is determined by

$$0=H(0)=1+JG_0(0)-\frac{3\pi^2}{16}\left(\frac{J\rho}{N}\right)^2. \quad (40)$$

Using (39) we see that

$$T_K'=\frac{2\gamma D}{\pi}\exp\left\{\frac{N}{J\rho}\left[1-\frac{3\pi^2}{16}\left(\frac{J\rho}{N}\right)^2\right]\right\} \quad (41)$$

or

$$T_K'=T_Ke^{-(3\pi/16)(J\rho^2/N)}>T_K \quad (42)$$

since $J<0$.

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New Solution for Exchange Scattering in Dilute Alloys

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The *s-d* exchange model is treated using equations of motion truncated at the lowest nontrivial order, following Nagaoka. The coupled equations are reduced to a single nonlinear integral equation for the conduction-electron t matrix, which depends only on energy. An approximation to the integral operator which treats the Kondo divergence accurately permits this equation to be transformed to a differential equation which is exactly integrable. The solution agrees with the leading terms of perturbation calculations above the Kondo critical temperature T_K, and passes through this temperature smoothly, reaching the unitarity limit at zero temperature. A different analytic continuation of the t matrix is trivially found which acquires nonphysical singularities below T_K. At low temperatures this form is shown to be identical to Abrikosov's solution and to Suhl's solution prior to analytic continuation. The resistivity of dilute alloys is calculated. Noninteracting impurities are shown to give no contribution to the specific heat. The effective local moment entering the magnetic susceptibility is found to be almost completely canceled at zero temperature for spin-$\frac{1}{2}$ impurities.

I. INTRODUCTION

SINCE Kondo's discovery of the low-temperature divergence in the perturbation series for conduction-electron scattering in dilute magnetic alloys,[1] a great deal of effort has been expended toward a physical understanding and an accurate calculation of the low-temperature properties of these systems. Unfortunately, a unified picture has not yet emerged. This work represents a "second generation" effort, yielding a new solution for the *s-d* exchange model which is simple,

[1] J. Kondo, Progr. Theoret. Phys. (Kyoto) 32, 37 (1964).