Low-Temperature Spin Correlations about a Localized Magnetic Impurity Moment*†

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The interaction of a localized impurity magnetic moment interacting with an electron gas by means of the *s-d* exchange interaction leads to the Kondo spin-compensated state at low temperatures, in which the moment of the impurity is greatly reduced. We have examined the electron-spin–impurity-spin correlation function in the ground state of the Nagaoka theory as well as those of the singlet theories due to Heeger and Jensen and to Kondo and Appelbaum. It is shown that the dominant behavior of the spin correlation function is given by $(\sin^2 k_F r)/(k_F r)^2$. It is also shown that the size of the spin-compensated state is characterized by a length ξ, which is inversely proportional to the energy parameter T_K in the Nagaoka theory, and to the binding energy ϵ of the singlet states in the singlet theories.

I. INTRODUCTION

THE problem of a localized-magnetic impurity has attracted considerable attention since Kondo's explanation of the resistivity minimum in 1964.[1] The breakdown of perturbation theory at temperatures below the Kondo temperature T_K led many workers to the use of self-consistent schemes,[2–4] such as a decoupling approximation in the equations of motion,[4] which have generated solutions to the problem at low temperatures. Unfortunately not very much information about the ground state of the localized moment-electron system has been obtained from these solutions. The work of Nagaoka[5] and Hamann,[6] on the susceptibility, however, seems to suggest the impurity spin is greatly reduced in the ground state. This last result involves a self-consistent decoupling procedure in addition to the original decoupling used by Nagaoka .[4]

The notion of a spin-compensated ground state has naturally led to the use of variational methods in which, for impurity spin $\frac{1}{2}$, the ground state has been described by a many-body singlet wave function,[7–10] thereby assuming complete compensation of the impurity spin. What these variational methods achieve is a ground state energy lower than that of the noninteracting system by an amount, ϵ, which is nonanalytic in the coupling, $\gamma=J\rho/N$, where J is the "$s-d$" interaction constant, ρ the density of states at the Fermi surface, and N the number of ions. The energy ϵ is similar in form to T_K, the Kondo temperature.

In order to get a deeper insight into the nature of the ground state predicted by the Nagaoka equations,[4] we shall examine the correlation between the conduction electrons and the localized impurity moment as given by the matrix element $\langle C_{k\uparrow}^{\dagger}C_{k'\uparrow}S_z\rangle$ which measures this correlation in momentum space. Because of symmetry considerations in spin space, this is related to the matrix element $\sum_{\alpha,\beta}(\mathbf{S}\cdot\boldsymbol{\sigma}_{\alpha\beta})C_{k\alpha}^{\dagger}C_{k'\beta}$ which, when transformed into real space, is a measure of the spin distribution of the electron cloud around the impurity. In momentum space this matrix element is a measure of the distortion of the Fermi surface in the particular ground state in question.

We shall compute $\langle C_{k\uparrow}^{\dagger}C_{k'\uparrow}S_z\rangle$ for the Nagaoka equations, the solution of which is due to Bloomfield and Hamann (BH),[11] as well as the variational methods of Heeger and Jensen (HJ),[7] and Kondo and Appelbaum (KA).[8] In addition the function $\bar{p}(\mathbf{r})\equiv\langle\mathbf{S}\cdot\boldsymbol{\sigma}(\mathbf{r})\rangle$ will be computed in all cases with the point of view of distinguishing the different theories.

II. NAGAOKA THEORY

In the Nagaoka formalism[4] one is able to write the electron propagator, $G_{kk'}(\omega)$, and the electron-impurity propagator, $\Gamma_{kk'}(\omega)$, as

$$G_{kk'}(\omega)=G_k^0(\omega)\delta_{kk'}+G_k^0(\omega)t(\omega)G_{k'}^0(\omega), \tag{1a}$$

$$\Gamma_{kk'}(\omega)=G_k^0(\omega)G_{k'}^0(\omega)\{(J/2N)[m_{k'}-S(S+1)]\times[1-\pi i\rho t(\omega)]+2t(\omega)[n_{k'}-\tfrac{1}{2}]\}, \tag{1b}$$

where $G_k^0(\omega)=(\omega-\epsilon_k)^{-1}$, ϵ_k being the electron kinetic energy measured relative to the Fermi surface, and $m_{k'}$ and $n_{k'}$ are defined as

$$n_{k'}=\sum_l\langle C_{l\uparrow}^{\dagger}C_{k'\uparrow}\rangle, \tag{2a}$$

$$m_{k'}=3\sum_l\langle C_{l\uparrow}^{\dagger}C_{k'\downarrow}S_-\rangle, \tag{2b}$$

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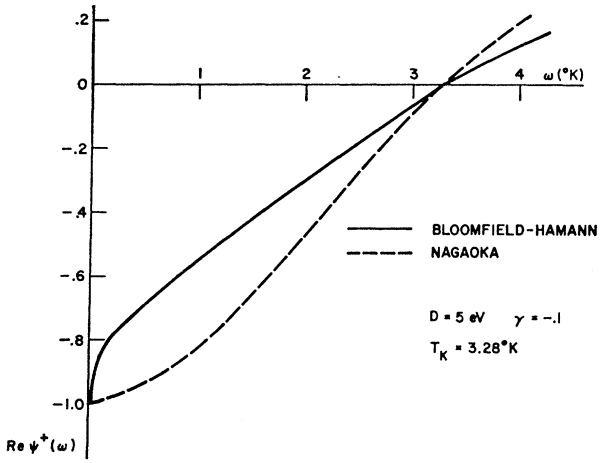

FIG. 1. The real part of the S matrix, $\psi^+(\omega)$, at $T=0°K$, as a function of ω. The dashed curve is the Nagaoka non-spin-flip solution and the solid curve is the exact solution of Bloomfield-Hamann.

while $t(\omega)$ is the non-spin-flip t matrix. The Nagaoka equations (1) are arrived at by assuming only the electron-impurity correlations are of importance and ignoring higher-order correlations, such as electron-electron correlations.

The Nagaoka approximation[4] implies an equation for the t matrix which may be most easily written by first defining the analog to the S matrix of scattering theory, $\psi(\omega)$, as

$$\psi(\omega)=1-2\pi i\rho t(\omega). \tag{3}$$

Then $\psi(\omega)$ obeys the equation[6,12]

$$\psi^+(\omega)=X^+(\omega)/[a+\phi_1{}^+(\omega)], \tag{4a}$$

$$\phi_1{}^+(\omega)=\int_{-D}^{D}d\omega'\frac{f(\omega')-\frac{1}{2}}{\omega-\omega'+i\eta}\phi^-(\omega'), \tag{4b}$$

where

$$X^+(\omega)=b+\int_{-D}^{D}d\omega'\frac{f(\omega')-\frac{1}{2}}{\omega-\omega'+i\eta}, \tag{5a}$$

$$b=\gamma^{-1}[1-S(S+1)(\tfrac{1}{2}\pi\gamma)^2], \tag{5b}$$

and

$$a=\gamma^{-1}[1+S(S+1)(\tfrac{1}{2}\pi\gamma)^2]. \tag{6}$$

Here $f(\omega)$ is the Fermi function, $\gamma=J\rho/N$ the dimensionless coupling constant, and the superscript on ϕ_1, X, and ψ indicates the function involved is the boundary value of a function holomorphic in one half of the complex ω plane; the symbol + means analytic in the upper half plane. Equation (4) has been solved by Bloomfield and Hamann (BH)[11]; the solution is

$$\psi^+(\omega)=\frac{-X^+(\omega)}{[[X^+(\omega)]^2+S(S+1)\pi^2]^{1/2}}\frac{1}{|K(\omega)|^{1/2}}\times\exp\left\{\frac{1}{2\pi i}P\int_{-D}^{D}d\omega'\frac{\ln|K(\omega')|}{\omega-\omega'}\right\}, \tag{7}$$

[12] D. S. Falk and M. Fowler, Phys. Rev. 158, 567 (1967).

with the function $K(\omega)$ being given by the relation

$$K(\omega)=\frac{X^+(\omega)X^-(\omega)+S(S+1)\pi^2}{[X^+(\omega)]^2+S(S+1)\pi^2}. \tag{8}$$

The details of the derivation and solution of these equations may be found in Refs. 4, 12, 6, and 11.

We have programmed an IBM 7094 computer to evaluate $\psi^+(\omega)$. The real and imaginary parts of $\psi^+(\omega)$ are shown in Figs. 1 and 2 with $S=\frac{1}{2}$ at $T=0°K$. These are compared with the old Nagaoka non-spin-flip solution,[4] $\psi_N{}^+(\omega)$, where

$$\psi_N{}^+(\omega)=(\omega-i\Delta_0)/(\omega+i\Delta_0), \tag{9}$$

with Δ_0 to be identified as T_K. The Kondo temperature, T_K, is determined from the relation

$$\mathrm{Re}\{X^+(\omega=0)\}=0, \tag{10}$$

which gives

$$T_K=De^{-1/|b|}. \tag{11}$$

In addition we have taken $2D$, the bandwidth, as 10 eV, and $\gamma=-0.1$; this gives a value for T_K of 3.28°K.

As a first step in calculating $\langle C_{k\uparrow}{}^\dagger C_{k'\uparrow}S_z\rangle$ we need to know the matrix elements n_k and m_k, defined as

$$n_k=\sum_1\langle C_{1\uparrow}{}^\dagger C_{k\uparrow}\rangle \tag{12a}$$

and

$$m_k=3\sum_1\langle C_{1\uparrow}{}^\dagger C_{k\downarrow}S_-\rangle. \tag{12b}$$

In the usual way these are related to frequency integrals of the retarded electron propagator, $G_{kk'}(\omega)$, and the retarded electron-impurity propagator, $\Gamma_{kk'}(\omega)$:

$$n_k=-2\,\mathrm{Im}\int\frac{d\omega}{2\pi}f(\omega)\sum_1 G_{1k}(\omega), \tag{13a}$$

and

$$m_k=-4\,\mathrm{Im}\int\frac{d\omega}{2\pi}f(\omega)\sum_1\Gamma_{1k}(\omega). \tag{13b}$$

After some straightforward manipulation (keeping in mind that one may let $f(\omega)\to f(\omega)-\frac{1}{2}$ in all integrals involving $t(\omega)$[6]) one obtains

$$n_k-\tfrac{1}{2}=-(1/2\pi)\,\mathrm{Im}\{\zeta(\epsilon_k)\}, \tag{14a}$$

and

$$m_k-S(S+1)=(2/\pi^2\gamma)\,\mathrm{Re}\{\zeta(\epsilon_k)\}, \tag{14b}$$

where $\zeta(\epsilon_k)$ is given by

$$\zeta(\epsilon_k)=X^+(\epsilon_k)-X^-(\epsilon_k)/\psi^-(\epsilon_k). \tag{15}$$

We have plotted these functions at $T=0°K$ for $S=\frac{1}{2}$ in Figs. 3 and 4. On the same graph is plotted the Nagaoka non-spin-flip result; it is seen that the approxi-

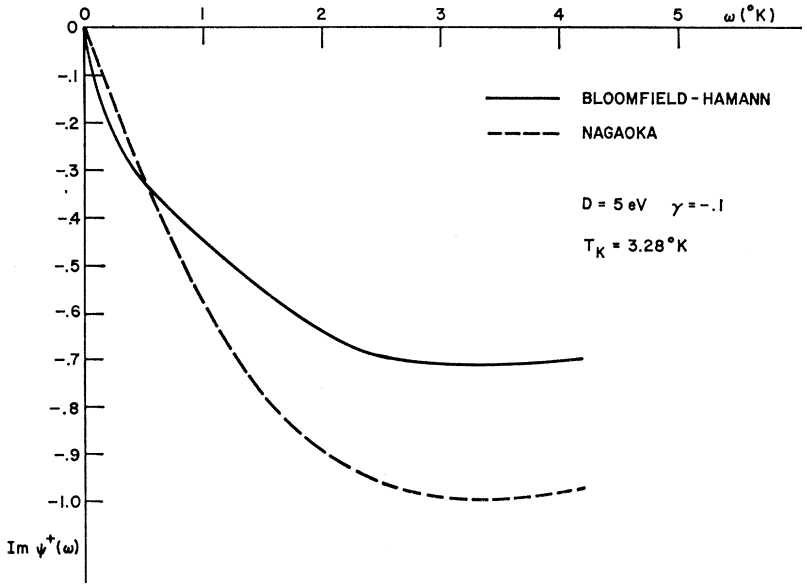

FIG 2. The imaginary part of the S matrix, $\psi^+(\omega)$, at $T=0°K$, as a function of ω. The dashed curve is the Nagaoka non-spin-flip solution and the solid curve is the exact solution of Bloomfield-Hamann.

mate Nagaoka results[4] approach their noninteracting values, zero and $-\frac{1}{2}$, respectively, more rapidly as the energy is increased than the exact solutions in BH.[11]

The primary purpose of this section is to compute $\langle C_{k\uparrow}^\dagger C_{k'\uparrow} S_z\rangle$. From the definition of $\Gamma_{kk'}(\omega)$ we have the formal expression

$$3\langle C_{k\uparrow}^\dagger C_{k'\uparrow} S_z\rangle = -2\,\mathrm{Im}\int \frac{d\omega}{2\pi} f(\omega)\Gamma_{kk'}(\omega). \quad (16)$$

Employing the identity

$$G_k^0(\omega)G_{k'}^0(\omega) = (1/(\epsilon_k-\epsilon_{k'}))\{G_k^0(\omega)-G_{k'}^0(\omega)\} \quad (17)$$

we rewrite (16) as

$$3\langle C_{k\uparrow}^\dagger C_{k'\uparrow} S_z\rangle = -\frac{1}{\pi}\frac{1}{\epsilon_k-\epsilon_{k'}}\,\mathrm{Im}\int d\omega\, f(\omega) \times\{[G_{k'}^0(\omega)]^{-1}-[G_k^0(\omega)]^{-1}\}\Gamma_{kk'}(\omega) \quad (18)$$

or

$$3\langle C_{k\uparrow}^\dagger C_{k'\uparrow} S_z\rangle \equiv A_{kk'}+B_{kk'}, \quad (19)$$

where $A_{kk'}$ and $B_{kk'}$ are two subsidiary functions defined such that $A_{kk'}$ corresponds to the first term in the integrand of (18), while $B_{kk'}$ corresponds to the second.

Thus our explicit expression for $A_{kk'}$ becomes

$$A_{kk'} = -\frac{1}{\pi}\frac{1}{\epsilon_k-\epsilon_{k'}}\,\mathrm{Im}\int d\omega \frac{f(\omega)}{\omega-\epsilon_k+i\eta} \times\{(J/2N)[m_{k'}-S(S+1)][1-\pi i\rho t(\omega)] +2[n_{k'}-\tfrac{1}{2}]t(\omega)\}. \quad (20)$$

If $f(\omega)\to f(\omega)-\frac{1}{2}$ in terms multiplying $t(\omega)$ in the integrand of (20), and $t(\omega)$ is then written in terms of $\psi(\omega)$ by means of (3), one has

$$A_{kk'} = -\frac{1}{\pi}\frac{1}{\epsilon_k-\epsilon_{k'}}\,\mathrm{Im}\int d\omega \frac{f(\omega)-\frac{1}{2}}{\omega-\epsilon_k+i\eta} \times\left\{(J/4N)[m_{k'}-S(S+1)][1+\psi^\dagger(\omega)] +\frac{1}{\pi i\rho}[n_{k'}-\tfrac{1}{2}][1-\psi^\dagger(\omega)]\right\} +\frac{1}{2}\frac{1}{\epsilon_k-\epsilon_{k'}}(J/2N)[m_{k'}-S(S+1)]. \quad (21)$$

By the definition of $A_{kk'}$ and $B_{kk'}$, (18) and (19), the form found for $\Gamma_{kk'}(\omega)$, (16), implies the last term of (21) will vanish in the sum $A_{kk'}+B_{kk'}$ so we will drop it. Then the definition of $\phi_2^\pm(\epsilon_k)$ as the complex conjugate of $\phi_1^\mp(\epsilon_k)$ [Eq. (46)] (see BH), combined with the definition of $X^\pm(\epsilon_k)$ [Eq. (5a)] gives

$$A_{kk'} \to -\frac{1}{\pi}\frac{1}{\epsilon_k-\epsilon_{k'}}(J/4N)[m_{k'}-S(S+1)] \times\mathrm{Im}\{-X^-(\epsilon_k)-\phi_2^-(\epsilon_k)\} -\frac{1}{\pi}\frac{1}{\epsilon_k-\epsilon_{k'}}\frac{1}{\pi\rho}(n_{k'}-\tfrac{1}{2}) \times\mathrm{Re}\{X^-(\epsilon_k)-b-\phi_2^-(\epsilon_k)\}, \quad (22)$$

or, by the definition of $\phi_2^-(\epsilon_k)$, we get

$$A_{kk'} \to 1/(\epsilon_k-\epsilon_{k'})(\gamma/2\rho) \times\{[m_{k'}-S(S+1)](n_k-\tfrac{1}{2})-m_k[n_{k'}-\tfrac{1}{2}]\}. \quad (23)$$

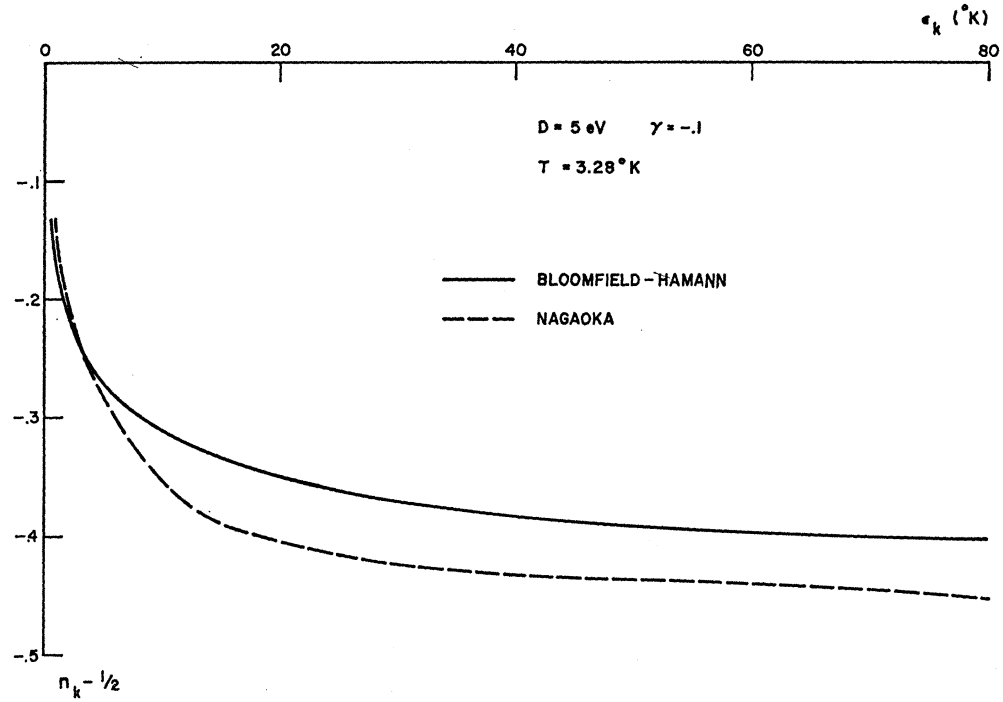

FIG. 3. The matrix element $n_k-\frac{1}{2}$ as a function of ϵ_k at $T=0$°K, for the Nagaoka and Bloomfield-Hamann solutions.

The evaluation of $B_{kk'}$ follows along the same lines. The result is

$$A_{kk'}+B_{kk'}=1/(\epsilon_k-\epsilon_{k'})(\gamma/2\rho)\times\{[n_k-\tfrac{1}{2}][m_{k'}-S(S+1)]-[n_{k'}-\tfrac{1}{2}][m_k-S(S+1)]\}, \quad (24)$$

so that

$$\langle C_{k\uparrow}{}^{\dagger}C_{k'\uparrow}S_z\rangle=(\gamma/6\rho)/(\epsilon_k-\epsilon_{k'})\times\{[n_k-\tfrac{1}{2}][m_{k'}-S(S+1)]-[n_{k'}-\tfrac{1}{2}][m_k-S(S+1)]\}. \quad (25)$$

The functions $n_{k'}-\frac{1}{2}$ and $m_{k'}-S(S+1)$ are odd and even in $\epsilon_{k'}$, respectively, since $X^+(\epsilon_k)=[X^+(-\epsilon_k)]^*$, and $\psi^+(\epsilon_k)=[\psi^+(-\epsilon_k)]^*$. Thus if we write

$$\langle C_{k\uparrow}{}^{\dagger}C_{k'\uparrow}S_z\rangle=(\gamma/6\rho)M(\epsilon_k,\epsilon_{k'}), \quad (26)$$

we have the relations

$$M(\epsilon_k,\epsilon_{k'})=M(\epsilon_{k'},\epsilon_k). \quad (27a)$$

M is even under the interchange of k and k', and

$$M(-\epsilon_k,-\epsilon_{k'})=M(\epsilon_k,\epsilon_{k'}), \quad (27b)$$

M is even under inversion with respect to the origin.

In Figs. 5 and 6 we have plotted $\langle C_{k\uparrow}{}^{\dagger}C_{k'\uparrow}S_z\rangle$ holding ϵ_k fixed and positive, and varying $\epsilon_{k'}$. From the limiting forms given in Appendix A, one may see that the

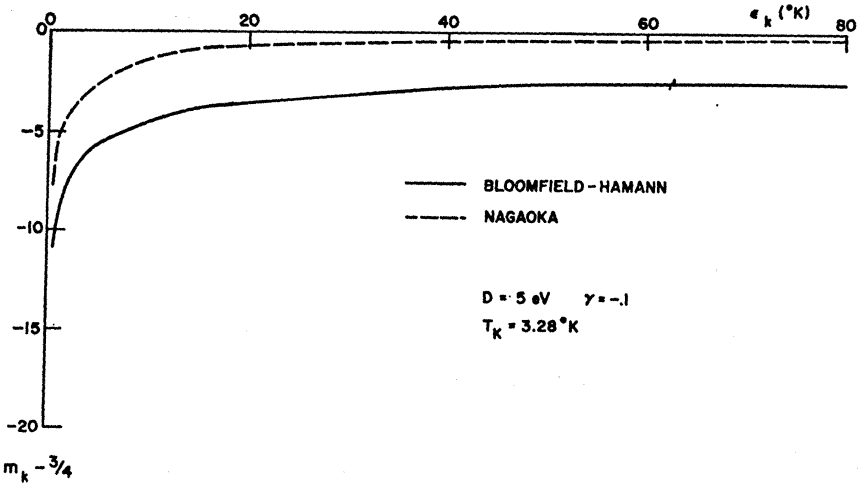

FIG. 4. The matrix element $m_k-\frac{3}{4}$ as a function of ϵ_k at $T=0$°K for the Nagaoka and Bloomfield-Hamann solutions.

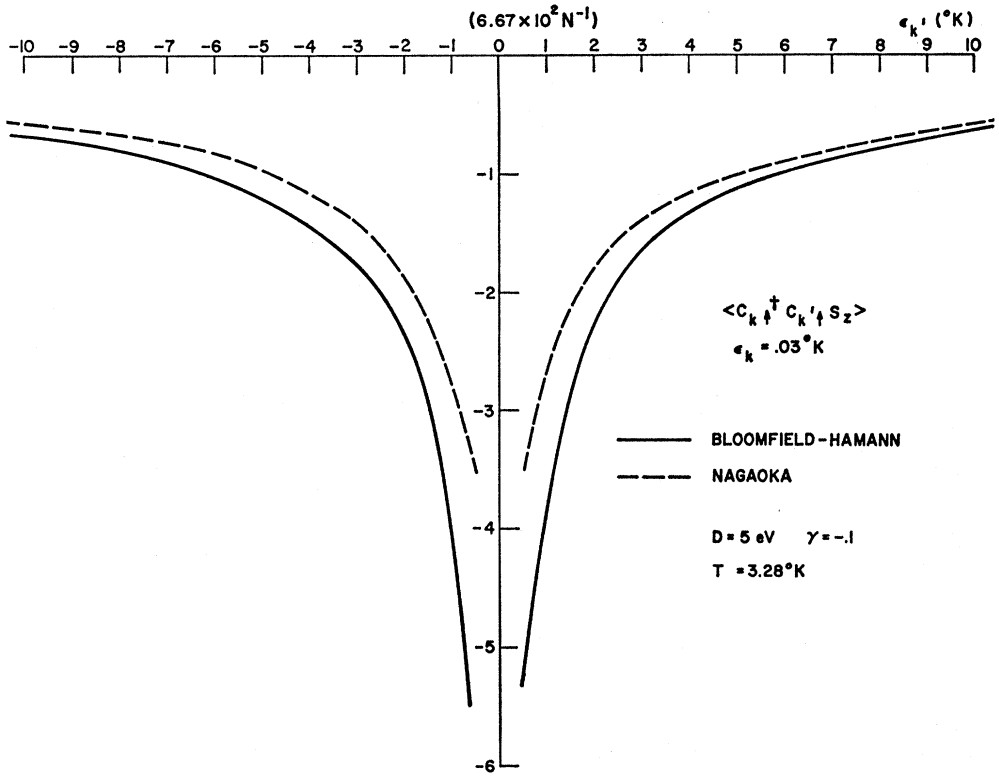

FIG. 5. The matrix element $\langle C_{k\uparrow}{}^{\dagger} C_{k'\uparrow} S_z \rangle$ at $T=0°\text{K}$ as a function of $\epsilon_{k'}$ with $\epsilon_k=0.03°\text{K}$.

matrix element diverges logarithmically when either ϵ_k or $\epsilon_{k'}$ are zero, i.e., on the Fermi surface. On the same graphs we have plotted the results of the Nagaoka approximate solution.[4] We notice the difference in the symmetry of the two solutions. This occurs because the function $M(\epsilon_k,\epsilon_{k'})$ in the Nagaoka non-spin-flip solution[4] is separable and proportional to $[m_k-S(S+1)] \times[m_{k'}-S(S+1)]$; thus $M^N(\epsilon_k,\epsilon_{k'})=M^N(\epsilon_k,-\epsilon_{k'})$.

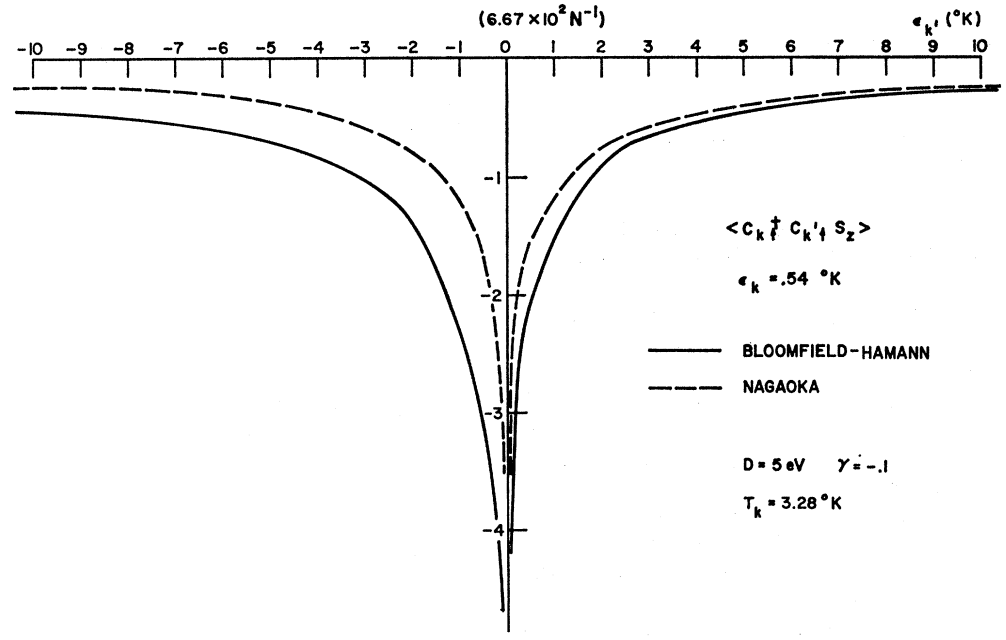

FIG. 6. The matrix element $\langle C_{k\uparrow}{}^{\dagger} C_{k'\uparrow} S_z \rangle$ at $T=0°\text{K}$ as a function of $\epsilon_{k'}$ with $\epsilon_k=0.54°\text{K}$.

That the exact solution does not exhibit such symmetry is obvious from (25).

In what follows we will exploit the variation of $M(\epsilon_{\mathbf{k}},\epsilon_{\mathbf{k}'})$ as a function of $\epsilon_{\mathbf{k}}$ and $\epsilon_{\mathbf{k}'}$ to obtain an estimate of the range and oscillatory behavior of the function $\bar{p}(\mathbf{r})=\langle \mathbf{S}\cdot\boldsymbol{\sigma}(\mathbf{r})\rangle$. The electron-spin–impurity-spin correlation function, $\bar{p}(\mathbf{r})$, is given, in terms of the matrix element $\langle C_{k\uparrow}^{\dagger}C_{k'\uparrow}S_z\rangle$ by the relation

$$\bar{p}(\mathbf{r})=6\sum_{k,k'}\langle C_{k\uparrow}^{\dagger}C_{k'\uparrow}S_z\rangle e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{r}}. \tag{28}$$

This correlation function, $\bar{p}(r)$, is important in that it specifies the spin distribution of the electron cloud around the impurity spin.

Converting the sums in (26) to integrals over $\mathbf{k}$ and $\mathbf{k}'$, and performing the angular integrations, we get

$$\bar{p}(\mathbf{r})=\frac{3}{2\pi^4}\frac{1}{r^2}\int_0^\infty dk\,k\sin kr \times\int_0^\infty dk'k'\sin k'r\langle C_{k\uparrow}^{\dagger}C_{k'\uparrow}S_z\rangle. \tag{29}$$

The arguments used by Nagaoka in computing $\bar{p}(\mathbf{r})$ for his approximate solution are not applicable here. In that case $\langle C_{k\uparrow}^{\dagger}C_{k'\uparrow}S_z\rangle$ was a separable function; as is evident from (25) this is no longer the case. He obtained[4] $\bar{p}(\mathbf{r})\sim\sin^2k_Fr/(k_Fr)^2$, for $k_F^{-1}\ll r\ll v_F/T_K$.

Substituting (26) into (29) and changing variables to dimensionless energies ($Dv=k^2/2m-D$) in units of half the bandwidth, D (which we take equal to the chemical potential), (29) becomes

$$\bar{p}(\mathbf{r})=(\tfrac{3}{2})\gamma n\frac{1}{x^2}\int_{-1}^{1}dv\sin[(1+v)^{1/2}x] \times\int_{-1}^{1}dv'\sin[(1+v')^{1/2}x]DM(Dv,Dv'), \tag{30}$$

where $x=k_Fr$ and n is the average density of electrons of one spin. The function $M(Dv,Dv')$ varies most rapidly over regions near the Fermi surface, therefore we want to consider this region separately. The rapid variation of $M(Dv,Dv')$ is over energies on the order of $V_K=T_K/D\ll1$; accordingly the region $|v|$, $|v'|<V_K$ will be considered separately. In fact we shall show in Appendix B that the remainder of the region of integration gives only contributions to $\bar{p}(\mathbf{r})$ of order x^{-4}, which, for $x\gg1$, can be neglected compared with the contributions kept.

Because of the weak logarithmic divergence of the matrix element as v or $v'\to0$ (see Appendix A) within the region $|v|$, $|v'|<V_K$, we shall treat the two strips $|v|<\delta$ and $|v'|<\delta$ separately, deferring the discussion of these strips until later. Here $\delta\ll V_K\ll1$. Since $V_K=T_K/D\ll1$, $(1+v)^{1/2}\simeq1+\frac{1}{2}v$ throughout. Then (30) becomes

$$\bar{p}(\mathbf{r})=(\tfrac{3}{2}\gamma n)\frac{1}{x^2}\int dv \times[\sin x\cos(\tfrac{1}{2}vx)+\sin(\tfrac{1}{2}vx)\cos x]\int dv' \times[\sin x\cos(\tfrac{1}{2}v'x)+\sin(\tfrac{1}{2}v'x)\cos x]DM(Dv,Dv'). \tag{31}$$

The form taken by the arguments of the oscillating functions in the integrand of (31), in particular $\frac{1}{2}vx$ and $\frac{1}{2}v'x$, suggests that we first consider that region of x in which $\cos\frac{1}{2}vx\simeq1$ and $\sin(\frac{1}{2}vx)\simeq\frac{1}{2}vx$. Thus we restrict ourselves to regions of x such that

$$x\ll V_K^{-1}=D/T_K. \tag{32}$$

Then (31) yields

$$\bar{p}(\mathbf{r})=(\tfrac{3}{2})\gamma n\frac{1}{x^2}\Big\{\sin^2x\int dv\int dv'DM(Dv,Dv') +(\tfrac{1}{2})x\sin2x\int dv\int dv'vDM(Dv,Dv') +(\tfrac{1}{4})x^2\cos^2x\int dv\int dv'vv'DM(Dv,Dv')\Big\}. \tag{33}$$

Only the presence of the second and third terms on the right-hand side of (33) makes this different from Nagaoka's result for $\bar{p}(\mathbf{r})$. The second term

$$(\tfrac{1}{2})x\sin2x\int dv\int dv'vDM(Dv,Dv')$$

vanishes since $M(x,y)=M(-x,-y)$, (27b). The third term, while nonzero is small since we have

$$\left|\int dv\int dv'vv'DM(Dv,Dv')\right| \leq|V_K|^2\left|\int dv\int dv'DM(Dv,Dv')\right|$$

so the ratio of this term to the first term in (33) is

$$\text{Ratio}\sim(\tfrac{1}{4})|V_K^2x^2|\ll1,$$

the inequality being due to the region of x we are considering (32).

Thus, neglecting the third term of (33) we get

$$\bar{p}(\mathbf{r})=-|a|\sin^2x/x^2,\quad 1\ll x\ll D/T_K, \tag{34}$$

where $x=k_Fr$, and

$$a=(\tfrac{3}{2}\gamma n)\int dv\int dv'DM(Dv,Dv'). \tag{35}$$

This result is essentially the same as that of Nagaoka [see Eqs. (4.19) and (4.20) of Ref. 4].

We must now verify that the two excluded strips of integration, $|v|<\delta$, $|v'|<\delta$, do not materially alter the result. Consider first the region in which $|v|>\delta$, but $|v'|<\delta$; then using the limiting values displayed in Appendix A we must deal with an integral of the form

$$\int_{|v|>\delta} dv[\sin x+(\tfrac{1}{2}vx)\cos x]\frac{(n_k-\frac{1}{2})}{(Dv)}\int_{-\delta}^{\delta} dv' \times[\sin x+(\tfrac{1}{2}v'x)\cos x]\ln|Dv'/T_K|,$$

where n_k is to be evaluated at $\epsilon_k=vD$.

Noting that $n_k-\frac{1}{2}$ is an odd function of v and $\ln|Dv'/T_K|$ is even in v', we get for this integral

$$\sin^2 x\int_{|v|>\delta} dv\frac{(n_k-\frac{1}{2})}{Dv}\int_{-\delta}^{\delta} dv'\ln|Dv'/T_K|.$$

We thus obtain only a small correction, proportional to $\delta\ln\delta$, to the $\sin^2x/x^2$ behavior found previously. The result for the region $|v|<\delta$, $|v'|>\delta$ is the same.

The square defined by $|v|$, $|v'|<\delta\ll V_K$ can be handled by considering the limiting forms of $M(x,y)$ given in Appendix A since $\delta\ll V_K\ll 1$ we write $\sin[(1+v)^{1/2}x]\simeq\sin x$ so our result is proportional to $\sin^2x/x^2$ and we must only make sure the remaining coefficient is finite.

The coefficient involves the integral

$$\int_{-\delta}^{\delta} dv\frac{\operatorname{sgn}v}{\ln^2|Dv/T_K|}\int_{-\delta}^{\delta} dv'\frac{\ln|Dv'/T_K|}{v'-v} = \int_{-\delta}^{\delta} dv\frac{\operatorname{sgn}v}{\ln^2|Dv/T_K|}I(v),$$

where

$$I(v)=\left\{\ln|Dv/T_K|\ln\left|\frac{\delta-v}{\delta+v}\right|\right\}-f_1\left(\frac{\delta-v}{v}\right)+f_1\left(-\frac{\delta+v}{v}\right);$$

where $f_1(x)$ is the Spence function[13] defined by

$$f_1(x)=-\int_0^x\frac{\ln|1-y|}{y}dy.$$

One can then demonstrate that $I(v)$ goes as $\ln^2v$ as $v\to 0$ and as $\ln|\delta\pm v|$ as $v\to\pm\delta$. Thus the integrand, $\ln^{-2}v\,I(v)$, is well behaved at $v=0$ and diverges logarithmically at the end points, $\pm\delta$. The logarithmic divergence is integrable and so the result is just some finite number proportional to δ. Consequently the contribution to $\bar{p}(\mathbf{r})$ is proportional to δ and hence negligible.

We may thus conclude that, within the Nagaoka picture, $\bar{p}(\mathbf{r})$, given by (34) is a reasonable description of the electron-spin-impurity spin correlation function for distances r from the impurity such that $1/k_F\ll r\ll\xi_N\equiv v_F/T_K$. For $r\gg\xi_N=v_F/T_K$ a similar argument yields $\bar{p}(\mathbf{r})$ proportional to x^{-4} times an oscillating function of k_Fr. (This is briefly explained in Appendix C.)

[13] K. Mitchell, Phil. Mag. 40, 351 (1949).

III. SINGLET-STATE VARIATIONAL THEORIES

The calculation of $\bar{p}(\mathbf{r})$ and $\langle C_{k\uparrow}^\dagger C_{k'\uparrow}S_z\rangle$ in Sec. II was performed in the context of the Nagaoka theory. We now proceed to a calculation of $\langle C_{k\uparrow}^\dagger C_{k'\uparrow}S_z\rangle$ and $\bar{p}(\mathbf{r})$ using the ground-state wave functions of Heeger and Jensen (HJ),[7] and Kondo and Appelbaum (KA).[8] These wave functions, the easiest to manipulate, have provided the smallest (HJ) and largest (KA) value of the binding energy for the spin-correlated state. The many-body singlet of Yosida, whose energy lies between these extremes, is not considered.

The first variational scheme with which we shall deal was proposed by Heeger and Jensen.[7] They represent the impurity spin by Fermi operators which create electrons in a single orbital d shell state localized on the impurity. This is suggestive of the Anderson model with a large intra-atomic Coulomb interaction U. The HJ singlet is

$$|\psi\rangle=K\sum_{\mathbf{k}}\frac{p_k}{\sqrt{2}}(C_{k\uparrow}^\dagger d_\downarrow^\dagger-C_{k\downarrow}^\dagger d_\uparrow^\dagger)\times\prod_{q\neq k}(U_q+f_qC_{q\uparrow}^\dagger C_{q\downarrow}^\dagger)|0\rangle, \quad (36)$$

where K is a normalization constant and p_k, U_k, and f_k are numbers to be determined variationally. The operators $d_\sigma^\dagger$ create electrons of spin σ in the localized d state, while the $C_{k\sigma}^\dagger$ create conduction electrons of momentum $\mathbf{k}$, spin σ.

The results for p_k, f_k, U_k, obtained by minimizing the energy in the state $|\psi\rangle$, are

$$f_k=(1-p_k^2)^{1/2},\ |\mathbf{k}|<k_F$$
$$=0,\qquad |\mathbf{k}|>k_F, \quad (37)$$
$$U_k=0,\qquad |\mathbf{k}|<k_F$$
$$=(1-p_k^2)^{1/2},\quad |\mathbf{k}|>k_F, \quad (38)$$

and

$$p_k^2=\frac{1}{2\rho\epsilon_{HJ}}\frac{1}{(1+|\epsilon_k|/\epsilon_{HJ})^2}, \quad (39)$$

where ρ is the density of states at the Fermi surface, ϵ_k the energy measured relative to the Fermi surface, and $-\epsilon_{HJ}$ is the reduction of the ground-state energy $\langle\psi|H|\psi\rangle/\langle\psi|\psi\rangle|_{\min}=E(J=0)-\epsilon_{HJ}$

$$\epsilon_{HJ}=De^{-4/3|\gamma|}. \quad (40)$$

Since the density of states, ρ, is proportional to the number of particles, N, divided by the Fermi energy, the pairing function p_k^2 is proportional to $1/N$; this is because there is only one impurity and only one electron

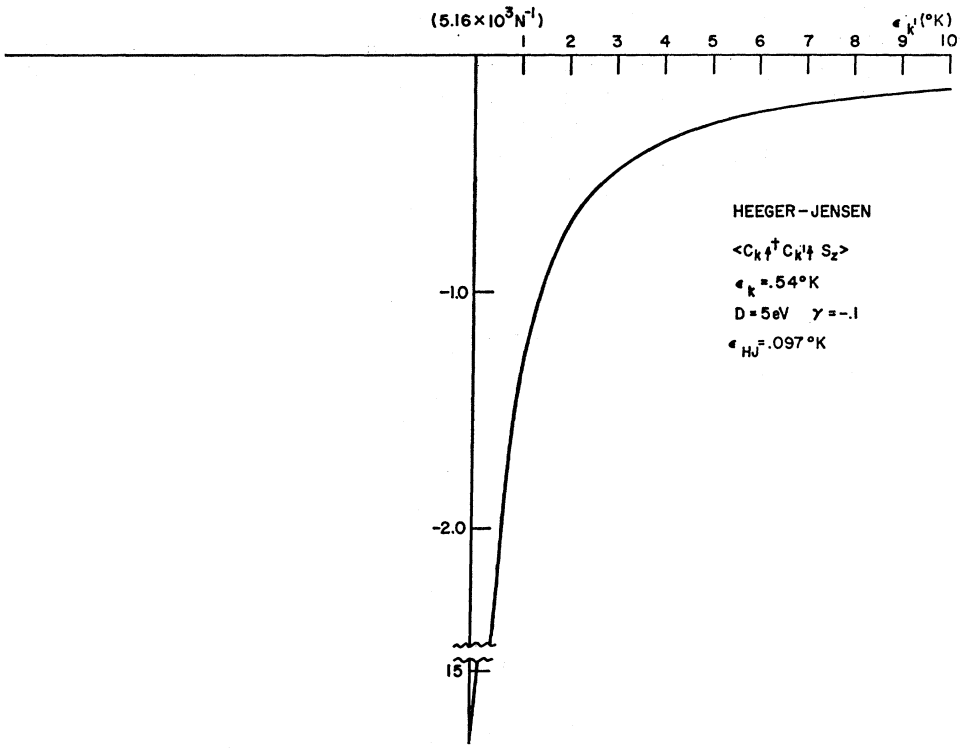

FIG. 7. The matrix element $\langle C_{k\uparrow}^{\dagger}C_{k'\uparrow}S_z\rangle$ in the Heeger-Jensen ground state as a function of $\epsilon_{k'}$ with $\epsilon_k=0.54°K$. The function is zero for $\epsilon_{k'}<0$ and has a finite value at the origin.

is used in forming the singlet. The functions f_k^2 and U_k^2 are analogous to Fermi functions for electrons and holes, respectively.

The matrix element $\langle C_{k\uparrow}^{\dagger}C_{k'\uparrow}S_z\rangle$ is computed in a straightforward fashion using (37). The result is

$$\langle C_{k\uparrow}^{\dagger}C_{k'\uparrow}S_z\rangle=-(\tfrac{1}{4})p_k p_{k'}(U_kU_{k'}+f_kf_{k'}) \quad (41)$$

plus terms of order $1/N^2$. Substituting the appropriate quantities we get

$$\langle C_{k\uparrow}^{\dagger}C_{k'\uparrow}S_z\rangle=-\frac{1}{8\rho\epsilon_{HJ}}\frac{1}{1+|\epsilon_k|/\epsilon_{HJ}}\frac{1}{1+|\epsilon_{k'}|/\epsilon_{HJ}}\times(f_kf_{k'}+U_kU_{k'}). \quad (42)$$

We shall ignore the deviation (of order $1/N$) of f_k and U_k from unity in the regions defined and make the approximations

$$f_k\simeq\theta(k_F-|\mathbf{k}|) \quad (43)$$

and

$$U_k\simeq\theta(|\mathbf{k}|-k_F).$$

Thus (42) becomes

$$\langle C_{k\uparrow}^{\dagger}C_{k'\uparrow}S_z\rangle=-\frac{1}{8\rho\epsilon_{HJ}}\frac{1}{1+|\epsilon_k|/\epsilon_{HJ}}\frac{1}{1+|\epsilon_{k'}|/\epsilon_{HJ}}\times\{\theta(k_F-|\mathbf{k}|)\theta(k_F-|\mathbf{k}'|)+\theta(|\mathbf{k}|-k_F)\theta(|\mathbf{k}'|-k_F)\}. \quad (44)$$

We note that $\mathbf{k}$ and $\mathbf{k}'$ must both either be above or below the Fermi surface; however the process where $\mathbf{k}$ is above the Fermi surface and $\mathbf{k}'$ below is not allowed. We have plotted $\langle C_{k\uparrow}^{\dagger}C_{k'\uparrow}S_z\rangle$ holding ϵ_k fixed and varying $\epsilon_{k'}$ in Fig. 7. The variation near $\epsilon_{k'}$ is much more rapid than was the case previously in BH; part of the reason for this is the scale of energies are very different, i.e., $\epsilon_{HJ}\ll T_K$. In addition we should point out that $\langle C_{k\uparrow}^{\dagger}C_{x'\uparrow}S_z\rangle$ does not have the logarithmic divergence that the BH result has as ϵ_k or $\epsilon_{k'}\to 0$.

The calculation of $\bar{p}(\mathbf{r})$ follows from (29) and (44). We find

$$\bar{p}(\mathbf{r})=-\left(\frac{9}{2}\frac{\epsilon_{HJ}}{n\epsilon_F}\right)\frac{1}{x^2}\sum_{j=1}^{2}[I(j)]^2, \quad (45)$$

where $x=k_Fr$, and $I(j)$ is given by

$$I(j)=\int_0^{\infty}\Omega_j dl\, l\sin lx\frac{1}{|l^2-1|+\epsilon_{HJ}/\epsilon_F}, \quad (46)$$

where

$$\Omega_1=1,\ l<1\quad \Omega_2=\begin{cases}0, & l<1\\ 0, & l>1;\end{cases}\quad =\begin{cases}0, & l<1\\ 1, & l>1.\end{cases} \quad (47)$$

The evaluation of $I(j)$ is straightforward. Since

$(\epsilon_{HJ}/\epsilon_F)\ll 1$ we get

$$I(1)=-\tfrac{1}{2}\cos[x+x\epsilon_{HJ}/2\epsilon_F]\times\{\mathrm{Si}[2x+x\epsilon_{HJ}/2\epsilon_F]-\mathrm{Si}[x\epsilon_{HJ}/2\epsilon_F]\}-\tfrac{1}{2}\sin[x+x\epsilon_{HJ}/2\epsilon_F]\times\{\mathrm{Ci}[x\epsilon_{HJ}/2\epsilon_F]-\mathrm{Ci}[2x+x\epsilon_{HJ}/2\epsilon_F]\}, \quad (48)$$

and

$$I(2)=\tfrac{1}{2}\cos[x-x\epsilon_{HJ}/2\epsilon_F]\times\{\pi-(\mathrm{Si}[x\epsilon_{HJ}/2\epsilon_F]+\mathrm{Si}[2x-x\epsilon_{HJ}/2\epsilon_F])\}+\tfrac{1}{2}\sin[x-x\epsilon_{HJ}/2\epsilon_F]\times\{\mathrm{Ci}[2x-x\epsilon_{HJ}/2\epsilon_F]-\mathrm{Ci}[x\epsilon_{HJ}/2\epsilon_F]\}. \quad (49)$$

We now want to consider these expressions for the range of x such that $1\ll x\ll\xi_{HJ}k_F$, where ξ_{HJ} is some characteristic length. We choose

$$\xi_{HJ}=v_F/\epsilon_{HJ} \quad (50)$$

so that, in this limit,

$$I(1)\underset{k_F^{-1}\ll r\ll\xi_{HJ}}{\sim}(-\pi/4)\cos x+(\tfrac{1}{2})\ln\left(\frac{\gamma_E x\epsilon_{HJ}}{2\epsilon_F}\right)\sin 2x, \quad (51)$$

where $\ln\gamma_E=0.577$ is Euler's constant, and

$$I(2)\underset{k_F^{-1}\ll r\ll\xi_{HJ}}{\sim}(\pi/4)\cos x-(\tfrac{1}{2})\ln\left(\frac{\gamma_E x\epsilon_{HJ}}{2\epsilon_F}\right)\sin x. \quad (52)$$

The $\ln x$ term multiplying $\sin x$ comes from the structure of the matrix element near the Fermi surface. Its magnitude is monotonically increasing as x becomes small and since $(\gamma_E x\epsilon_{HJ}/\epsilon_F)\ll 1$, it is expected to dominate the factor $\pi/4$ multiplying $\cos x$. Upon performing the required manipulations

$$\bar{p}(\mathbf{r})\underset{k_F^{-1}\ll r\ll\xi_{HJ}}{\sim}-\left(\frac{9}{2}\frac{\epsilon_{HJ}}{n\epsilon_F}\right)\frac{1}{x^2}\times\left\{\frac{\pi^2}{16}\cos^2 x+(\tfrac{1}{4})\ln^2\left(\frac{\gamma_E\epsilon_{HJ}x}{2\epsilon_F}\right)\sin^2 x\right\}. \quad (53)$$

It is relatively easy to see that $\bar{p}(\mathbf{r})\to x^{-4}$ for $x\gg\xi_{HJ}k_F$. Since, for a fixed value of γ, the T_K of the Nagaoka theory is larger than ϵ_{HJ}, the characteristic length, $\xi_{HJ}\simeq v_F/\epsilon_{HJ}$, is correspondingly longer.

The lowest ground state energy obtained in a variational theory to date has been in the work of Kondo and Appelbaum.[8] Although similar in concept to HJ, their wave functions builds up the many body singlet by using combinations of free electron operators.

The KA wave function is

$$|\psi\rangle=\tfrac{1}{2}\sqrt{2}(a_{0\uparrow}^{\dagger}\beta-a_{0\downarrow}^{\dagger}\alpha)\prod_{l=1}^{N/2}a_{l\uparrow}^{\dagger}a_{l\downarrow}^{\dagger}|0\rangle, \quad (54)$$

where α and β are the usual spin-up and spin-down spinors for the impurity and the operators $a_{l\sigma}^{\dagger}$ create a particle in the state l with spin σ. The a's are defined in terms of the usual electron operators, $C_{k\sigma}^{\dagger}$, by means of a, to be determined, cannonical transformation.

$$a_{0\sigma}^{\dagger}=\sum_k p_{0k}C_{k\sigma}^{\dagger}, \quad (55a)$$

$$a_{l\sigma}^{\dagger}=\sum_k p_{lk}C_{k\sigma}^{\dagger}. \quad (55b)$$

This wave function, as that in (36), attempts to represent the spin condensed part of the ground state by the operator a_0 while the Fermi sea, suitably modified, is built up by the other a's. The variational calculation then proceeds to find p_{0k} and from it p_{lk} (they are not independent since the conditions of the canonical transformation require $\sum_k p_{0k}p_{lk}^{\dagger}=0$). The form of p_{0k} is determined only approximately by an integral equation obtained by minimizing the expectation value of the Hamiltonian with respect to the p's, and is assumed from its large energy behavior to be

$$p_{0k}=\left(\frac{1}{2\rho\epsilon}\right)^{1/2}\frac{1}{1+|\epsilon_k|/\epsilon}. \quad (56)$$

The parameter ϵ is then found by minimizing E and has the same significance as in HJ, i.e.,

$$\langle\psi|H|\psi\rangle/\langle\psi|\psi\rangle|_{\min.}=E(J=0)-\epsilon_{KA},$$

with

$$\epsilon_{KA}=De^{-2/3|\gamma|}. \quad (57)$$

We notice that for a fixed value of γ this turns out to be considerably larger than both ϵ_{HJ} and T_K. Since the trial wave function, (50), does not provide that p_{0k} exactly satisfy the integral equation derived from this formalism, the true energy $-\epsilon$ could be even lower and $-\epsilon_{KA}$ is an upper bound:

$$-\epsilon\leq-\epsilon_{KA}.$$

We next compute $\langle C_{k\uparrow}^{\dagger}C_{k'\uparrow}S_z\rangle$ and the spin correlation function, $\bar{p}(\mathbf{r})$. Using (54), the inverse of (55), and (56), we find

$$\langle C_{k\uparrow}^{\dagger}C_{k'\uparrow}S_z\rangle=-\frac{1}{8\rho\epsilon_{KA}}\frac{1}{1+|\epsilon_k|/\epsilon_{KA}}\frac{1}{1+|\epsilon_{k'}|/\epsilon_{KA}}. \quad (58)$$

We notice that the form of $\langle C_{k\uparrow}^{\dagger}C_{k'\uparrow}S_z\rangle$ in KA is the same as that due to HJ, (44), to order $1/N$, There is, of course, the definition of ϵ, which differs radically in magnitude in the two cases; but more significant is the fact that the KA result (58) does not distinguish between above and below the Fermi surface as does HJ, (44). We have plotted $\langle C_{k\uparrow}^{\dagger}C_{k'\uparrow}S_z\rangle$ in Fig. 8 holding ϵ_k fixed and varying $\epsilon_{k'}$. The range of variation here is over a much larger energy range since $\epsilon_{KA}\gg T_K$, ϵ_{HJ}. As with HJ, the KA result has a finite value as $\epsilon_{k'}\to 0$. However the distortion of the Fermi surface is so great in KA that the density of states is now infinite there.

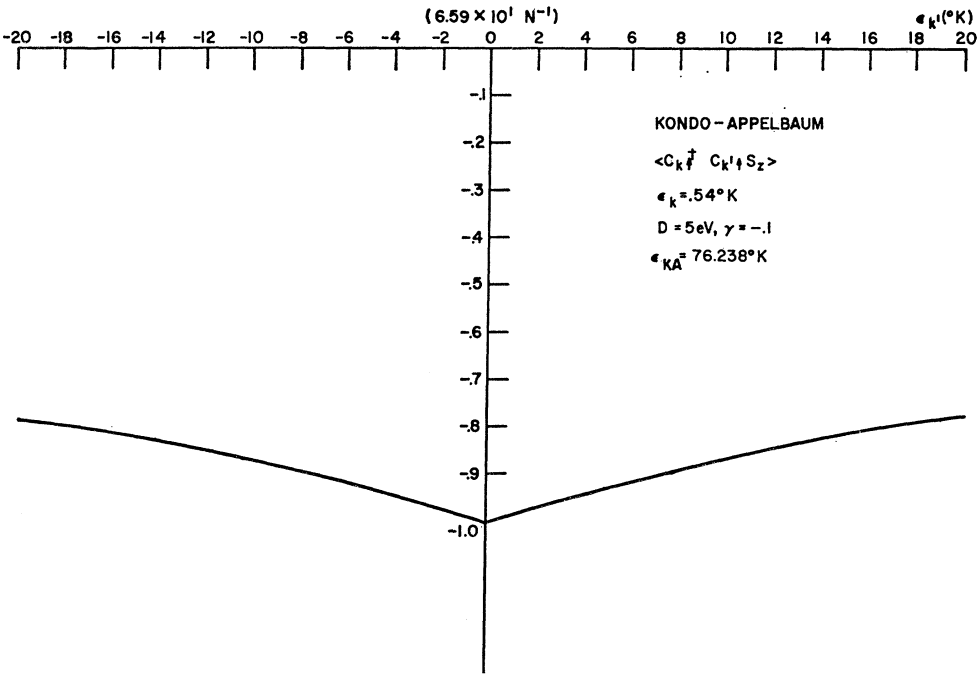

FIG. 8. The matrix element $\langle C_{k\uparrow}{}^{\dagger}C_{k'\uparrow}S_z\rangle$ in the Kondo-Appelbaum ground state as a function of $\epsilon_{k'}$ with $\epsilon_k=0.54°\text{K}$. The function has a finite value at $\epsilon_{k'}=0$.

The calculation of $\bar{p}(\mathbf{r})$ follows directly from the HJ calculation. In this case, however, there are no θ function restrictions. Consequently it is easy to get

$$\bar{p}(\mathbf{r})=-\left(\frac{9}{2}n\frac{\epsilon_{\mathrm{KA}}}{\epsilon_F}\right)\frac{1}{x^2}[I(1)+I(2)]^2, \tag{59}$$

where $I(j)$ are identical to those defined in (46) and (47), except that ϵ_{KA} replaces ϵ_{HJ}. Using the limiting values given in (51) and (52) we conclude that

$$I(1)+I(2)\underset{k_F^{-1}\ll r\ll\xi_{\mathrm{KA}}}{\sim}-\sin x\ln\frac{\gamma_E\epsilon_{\mathrm{KA}}}{2\epsilon_F}x, \tag{60}$$

where ξ_{KA} is similar to ξ_{HJ} but ϵ_{KA} has replaced ϵ_{HJ},

$$\xi_{\mathrm{KA}}=v_F/\epsilon_{\mathrm{KA}}. \tag{61}$$

Thus,[14]

$$\bar{p}(\mathbf{r})\underset{k_F^{-1}\ll r\ll\xi_{\mathrm{KA}}}{\sim}-\left(\frac{9}{2}n\frac{\epsilon_{\mathrm{KA}}}{\epsilon_F}\right)\frac{1}{x^2}\sin^2x\ln^2\frac{\gamma_E\epsilon_{\mathrm{KA}}x}{2\epsilon_F}. \tag{62}$$

The characteristic length here is much less than ξ_{HJ} since

$$\xi_{\mathrm{KA}}=v_F/\epsilon_{\mathrm{KA}}=(v_F/\epsilon_{\mathrm{HJ}})e^{-2/3|\gamma|}\ll\xi_{\mathrm{HJ}}.$$

[14] After completion of this work we received a report from Heeger, Welsh, Jensen, and Gladstone in which they have obtained essentially this form for $\bar{p}(\mathbf{r})$. We wish to thank them for sending us their work prior to publication. A. J. Heeger, L. B. Welsh, M. A. Jensen and G. Gladstone, Phys. Rev. **172**, 302 (1968).

For $x\gg\xi_{\mathrm{KA}}r$ the asymptotic expansions of $I(1)+I(2)$ go to zero faster than x^{-1}, so that $\bar{p}(\mathbf{r})=O(1/x^5)$ when $x\gg\xi_{\mathrm{KA}}r$.

IV. CONCLUSIONS

We have thus shown the similarity of the spatial dependence of the spin correlation function, $\bar{p}(\mathbf{r})$, in all the theories considered. The dominant behavior of $\bar{p}(\mathbf{r})$ is $(\sin^2k_Fr)/(k_Fr)^2$, a relatively long range function. This behavior is independent of the specific theory. In the singlet theories it is possible to evaluate $\bar{p}(\mathbf{r})$ exactly and, in those cases, we have found a slowly varying function of the form $\ln^2(r/\xi)$ multiplying the $(\sin^2k_Fr)/(k_Fr)^2$ term. Apparently this comes from the detailed structure of $\langle C_{k\uparrow}{}^{\dagger}C_{k'\uparrow}S_z\rangle$ near the Fermi surface and our treatment of the Nagaoka theory is insensitive to such details.

The characteristic length ξ in each case has the form v_F/ϵ, where ϵ is chosen from the appropriate theory; in this sense ξ is theory independent. This length, in each theory, corresponds to that distance from the impurity beyond which $\bar{p}(\mathbf{r})$ changes its behavior and falls off more rapidly. It may therefore be viewed as a measure of the "size" of the spin compensated state. Since ξ is inversely proportional to the binding energy ϵ we have the inequalities

$$\xi_{\mathrm{KA}}\ll\xi_N\ll\xi_{\mathrm{HJ}},$$

since

$$\epsilon_{\mathrm{KA}}\gg\epsilon_N\equiv T_K\gg\epsilon_{\mathrm{HJ}}.$$

That is, the size of the correlated ground state is smaller as the binding is greater.

Note added in proof: Recently a different coherence length has been suggested.[15] We should like to point out that this length v_F/D is simply a measure of the change in total electron density in the vicinity of the impurity, and in fact only reflects the range of the potential. It has nothing to do with the range of the *spin* correlations, which reflects the properties of the spin compensated state.

APPENDIX A

In this appendix we wish to display the limiting forms for small energies of the functions found in Sec. II. We are only interested in the case $T=0°\mathrm{K}$ and thus, from (5a) and (10) we write

$$X^+(\omega)=-\ln|\omega/T_K|+(\tfrac{1}{2}i\pi)\,\mathrm{sgn}(\omega). \tag{A1}$$

For small ω our expansion will most naturally be in inverse powers of $\ln|\omega/T_K|$. The expansion of $\psi(\omega)$, (7), can easily be achieved using an approximate form found by Hamann[6]:

$$\psi_1^+(\omega)=\frac{-X^+(\omega)}{([X^+(\omega)]^2+S(S+1)\pi^2)^{1/2}}. \tag{A2}$$

This is permissible since $|K(\omega)|$ is an even function and so the integral

$$P\int_{-D}^{D}d\omega'\frac{\ln|K(\omega')|}{\omega-\omega'}$$

yields only odd powers of ω which go to zero much more rapidly than the inverse $\ln|\omega/T_K|$ dependence of $\psi_1^+(\omega)$. The term $|K(\omega)|^{-1/2}$ is dropped because $|K(\omega)|\to 1+O(\ln^{-3}|\omega/T_K|)$, as $\omega/T_K\to 0$. Then we have

$$\mathrm{Re}\psi^+(\omega)\underset{|\omega|/T_K\to 0}{\sim}-1+\frac{\frac{1}{2}\pi^2}{\ln^2|\omega/T_K|}, \tag{A3}$$

and

$$\mathrm{Im}\psi^+(\omega)\underset{|\omega|/T_K\to 0}{\sim}\frac{\frac{3}{8}\pi^2\,\mathrm{sgn}(\omega)}{\ln^3|\omega/T_K|}. \tag{A4}$$

Substituting (A3) and (A4) into (13) yields the limiting forms

$$n_k-\tfrac{1}{2}\underset{|\epsilon_k|/T_K\to 0}{\sim}\frac{-\pi^2}{16}\frac{\mathrm{sgn}(\epsilon_k)}{\ln^2|\epsilon_k/T_K|}, \tag{A5}$$

and

$$m_k-S(S+1)\underset{|\epsilon_k|/T_K\to 0}{\sim}\frac{4}{\pi^2|\gamma|}\ln|\epsilon_k/T_K|. \tag{A6}$$

Consequently we find from (25) that $\langle C_{k\uparrow}^\dagger C_{k'\uparrow}S_z\rangle$ becomes logarithmically infinite if either the electron destroyed, labeled $\mathbf{k}'$, or the electron created, labeled $\mathbf{k}$, is at the Fermi surface. Explicitly

$$\lim_{\substack{\epsilon_k\to 0\\ \epsilon_{k'}\text{ arbitrary}}}\langle C_{k\uparrow}^\dagger C_{k'\uparrow}S_z\rangle=\frac{\gamma}{6\rho}\frac{n_{k'}-\frac{1}{2}}{\epsilon_{k'}}\frac{4}{\pi^2|\gamma|}\ln|\epsilon_k/T_K|. \tag{A7}$$

APPENDIX B

In this section we will show that the contribution to $\bar{p}(\mathbf{r})$ from integrating over the region $|v|$, $|v'|>V_K$ is proportional to x^{-4}, and therefore, for $x\gg 1$, is negligible.

The integral is

$$\int dv\int dv'\,\sin[(1+v)^{1/2}x]\sin[(1+v')^{1/2}x]\times DM(Dv,Dv'). \tag{B1}$$

Our argument is the same for all four quadrants in the v, v' plane so we need only consider the region v, $v'>0$. In that case the integral in (B1) can be broken up as

$$\int_{V_K}^{1}dv\int_{V_K}^{1}dv'+\int_{0}^{V_K}dv\int_{V_K}^{1}dv'+\int_{V_K}^{1}dv\int_{0}^{V_K}dv'. \tag{B2}$$

In the region where $V_K<v,v'<1$, the function $M(Dv,Dv')$ is either zero or very slowly varying. Assuming the latter we replace $M(Dv,Dv')$ by some average value. Thus

$$\int_{V_K}^{1}dv\int_{V_K}^{1}dv'\to\bar{M}\int_{V_K}^{1}dv\int_{V_K}^{1}dv'\times\sin[(1+v)^{1/2}x]\sin[(1+v')^{1/2}x], \tag{B3}$$

where $\bar{M}$ is the average value of M in this region. Making the substitution $1-v=k^2$, the integration yields a term proportional to $\cos^2x/x^2$ and since, by (30), $\bar{p}(\mathbf{r})$ has an extra factor of x^{-2}, the contribution to $\bar{p}(r)$ from it is x^{-4}.

The argument for the remaining integrals applies to either so we only consider

$$\int_{V_K}^{1}dv\int_{0}^{V_K}dv'\,\sin[(1+v')^{1/2}x]\sin[(1+v)^{1/2}x]\times M(Dv,Dv'). \tag{B4}$$

We proceed by writing

$$\int_0^{V_K}dv'=\int_0^{\delta'}dv'+\int_{\delta'}^{V_K}dv',$$

where $\delta'\ll V_K=T_K/D$. In the case where we integrate v' from δ' to V_K the function $M(Dv,Dv')$ is slowly vary-

[15] A. Zawadowski and J. Solyom, in Proceedings of the Eleventh International Conference on Low Temperature Physics, St. Andrews, 1968 (unpublished) and, (to be published).

ing since $v>V_K$ even though $\delta'<v'<V_K$. Then the previous argument applies and we get a contribution proportional to x^{-2}, and a contribution to $\bar{p}(\mathbf{r})\sim x^{-4}$.

In the remaining integral, we write $(1+v')^{1/2}\simeq 1+\frac{1}{2}v'$, since $\delta'\ll 1$, and use the limiting form (A7) to get:

$$\int_{V_K}^{1} dv \sin[(1+v)^{1/2}x]\frac{n_k-\frac{1}{2}}{Dv}\int_0^{\delta'} dv' \times\{\sin x\cos\tfrac{1}{2}v'x+\sin\tfrac{1}{2}v'x\cos x\}\ln|Dv'/T_K|. \quad \text{(B5)}$$

Denoting the v' integral from 0 to δ' as I_1 we have

$$|I_1|\leq -2\int_0^{\delta'}\ln|Dv'/T_K|dv', \quad \text{(B6)}$$

so that

$$|I_1|\leq 2\delta'\left[\ln\frac{T_K}{D\delta'}+1\right]$$

and so this contribution to $\bar{p}(\mathbf{r})$ is small compared to the term we have kept, (34).

APPENDIX C

In this section we will demonstrate that $\bar{p}(\mathbf{r})\sim x^{-4}$, for $x/k_F\gg\xi_N=v_F/T_K$. By Appendix B we need only consider the region of integration $0<|v|$, $|v'|<V_K=T_K/D\ll 1$. Hence, we may take $(1+v)^{1/2}\simeq 1+\frac{1}{2}v$, but the linear approximations for $\sin vx/2$ and $\cos vx/2$ are no longer valid since $(\frac{1}{2}V_Kx)\gg 1$, for $x\gg V_K^{-1}=D/T_K$.

Our expressions for $\bar{p}(\mathbf{r})$, (30), then takes the form

$$\bar{p}(\mathbf{r})=\tfrac{3}{2}\gamma n\left\{\frac{\sin^2x}{x^2}\int dv\cos\tfrac{1}{2}vx\int dv'\cos\tfrac{1}{2}v'xDM(Dv,Dv')\right.$$
$$+\frac{\sin 2x}{x^2}\int dv\sin\tfrac{1}{2}vx\int dv'\cos\tfrac{1}{2}v'xDM(Dv,Dv')$$
$$\left.+\frac{\cos^2x}{x^2}\int dv\sin\tfrac{1}{2}vx\int dv'\sin\tfrac{1}{2}v'xDM(Dv,Dv')\right\}. \quad \text{(C1)}$$

The argument used previously when $x/k_F\ll\xi_N$ again serves to eliminate the term proportional to $\sin 2x$, the integrand still being odd with respect to inversion through the origin.

The limits of integration are $V_K=T_K/D\ll 1$; hence we can find some number $\zeta\ll V_K$ in which the linear approximations of Appendix B hold. The contribution from this section would be $\sin^2x/x^2$ but since $\zeta\ll V_K$ the weight of this contribution is accordingly very small.

Except for the strips $|v|<\zeta<|v'|$ and $|v'|<\zeta<|v|$, the period of the oscillating functions in the rest of the region, i.e., for $\zeta<|v|,|v'|<V_K$ is proportional to x^{-1}. Since $x^{-1}\ll V_K$, these functions oscillate very rapidly and this behavior dominates the variation of $M(Dv,Vv')$ in this region. Holding $M(Dv,Dv')$ at some constant value we obtain two extra powers of x^{-1}. Thus we have $\bar{p}(\mathbf{r})\sim(k_Fr)^{-4}$ times an oscillatory function of k_Fr. The strips mentioned above can be handled as in Sec. II and Appendix B and, as there, contribute little to the result.