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Effect of potential scattering on the low-temperature spin-fluctuation resistivity

D. J. Gillespie
Naval Research Laboratory, Washington, D. C. 20375
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We have evolved a spectral density function for the distribution of spin fluctuations, $A(q,\omega)$, which is expected to be valid for all values of q and ω for an exchange-enhanced system containing randomly distributed scattering centers. Using this function we have calculated the effect of the potential scattering on the magnitude of the coefficient of the T^2 term which occurs in the electrical resistivity of both uniformly and locally exchange-enhanced systems. Contrary to what might have been presumed, we find that potential scattering increases the T^2 term. In most cases this increase is a small fraction of the original T^2 term. For example, we calculate that the increase in the T^2 term in the spin-fluctuation resistivity of $Pd_{95}Rh_5$ will be only $\sim 2\%$ as a result of the potential scattering. Also, the increase in the additional T^2 contribution which results from the introduction of Ni into this alloy will also be only $\sim 2\%$ as a result of the potential scattering in the $Pd_{95}Rh_5$ host.

I. INTRODUCTION

The application of many-body techniques to explain the electronic properties of the nearly ferromagnetic metals Rh, Pd, and Pt and their alloys has greatly increased our understanding of these materials. Many of their electronic properties (e.g., magnetic susceptibility, specific heat, and electrical resistivity) can be accounted for by a model which explicitly includes a strong intra-atomic Coulomb interaction between the d-band electrons of opposite spin. For example, early theoretical work predicted that the intra-atomic Coulomb interaction would enhance the spin fluctuations in the d-band of these materials and that an enhanced T^2 term in the electrical resistivity at low temperatures would result[1–3] from conduction electrons scattering from these exchange-enhanced spin fluctuations. The good quantitative agreement between theory[3] and the experimental work[2] on the *Pd*Ni system seemed to confirm the validity of the model. However, the model also predicted that the addition of Rh to the *Pd*Ni system would lead to a further enhancement of the T^2 term, but recent experimental work[4–6] showed that this was not the case. One possible reason for the discrepancy between the prediction of the model and the results of the experiment is that the model has neglected the effect of the increased potential scattering that occurs as a result of the Rh addition. It is the effect of this potential scattering on the T^2 term in the spin-fluctuation resistivity that we discuss in this paper.

The strength of the exchange enhancement in these nearly ferromagnetic materials is reflected by the Stoner enhancement factor, which is defined as $S=\chi/\chi_0$, where χ is the experimentally determined static paramagnetic susceptibility and χ_0 is the "bare-band" susceptibility determined from the density of states. In the random-phase approximation the Stoner enhancement factor is given by[7] $S=1/[1-UN(E_F)]$ where U is a parameter which is a measure of the strength of the intra-atomic Coulomb interaction between the d-band electrons of opposite spin and $N(E_F)$ is the density of states at the Fermi level (E_F) per spin state per atom.

Of the nearly ferromagnetic metals Pd, Pt, and Rh and their alloys with each other, the alloy $Pd_{95}Rh_5$ has the highest magnetic susceptibility. The increase in the susceptibility of this alloy over that of pure Pd is thought[8] to be the result of the combination of two features: an increase in the density of states at the Fermi level, and a local enhancement of the susceptibility associated with the Rh sites. Thus, the alloy is expected to have a higher Stoner enhancement factor than Pd, since both the average interaction parameter U and the density of states are greater for the alloy. As a result of the increased enhancement, $Pd_{95}Rh_5$ might very well be expected to act as a superenhanced Pd, exhibiting strong spin-fluctuation effects. For example, the low-temperature T^2 term of the electrical resistivity of this alloy would be expected to be greater than that of Pd. Also, the addition of a dilute amount of Ni to a $Pd_{95}Rh_5$ alloy would be expected to yield even larger local enhancement effects than were found[2] for the addition of Ni to Pd. However, the experimentally determined T^2 coefficient of $Pd_{95}Rh_5$ is not larger than that of Pd; it is in fact negative.[9] Also, the addition of Ni to this alloy does not produce a larger increase in the T^2 term than does the addition of Ni to Pd; it produces only a comparable increase.[4–6]

It has been suggested[5] that one possible reason for a reduced T^2 term in the Pd-Rh system may be that the large amount of potential scattering that comes from the Rh atoms dampens the spin fluctuations and thereby reduces the magnitude of the T^2 contribution from spin fluctuations. However, there appears to have been no previous calculation of the effect that potential scattering will have on the T^2 term of a uniformly exchange-enhanced system.

In Sec. II we present such a calculation. First, we we use the model of Mills and Lederer[1] to obtain an expression for the T^2 term that appears in the low-temperature resistivity when conduction electrons scatter from spin fluctuations. In this model, s-band conduction electrons scatter from spin fluctuations in the d band via the s-d exchange interaction, and the coefficient of the T^2 term depends directly upon the energy-momentum distribution of the spin fluctuations. The effect of potential scattering on this T^2 coefficient is then calculated by using a distribution function which reflects the effect of potential scattering. For most phenomena one could use the dynamic susceptibility result of Fulde and Luther[10] to obtain a satisfactory distribution function. However, since the calculation of the coefficient of the T^2 term in the electrical resistivity involves a strong weighting of the high-momentum end of the distribution function, and since their result is valid only when the value of the momentum q is much less than the Fermi momentum of the d band, q_F, it seems unlikely that Fulde and Luther's result would give a realistic T^2 coefficient. We have therefore determined a more realistic distribution function which interpolates between (i) Fulde and Luther's distribution function (valid in the presence of potential scattering when $q \ll q_F$) and (ii) the random-phase-approximation distribution function[11] (valid for all q in the limit of no potential scattering). Using this interpolated distribution function (expected to be valid for all ranges of q in the presence of potential scattering), we calculate the effect of potential scattering upon the T^2 term in the spin-fluctuation resistivity for a uniformly exchange-enhanced system.

Finally, we consider a system consisting of a locally enhanced impurity in an exchange-enhanced host. Using the above-determined distribution function for the host along with the local-enhancement model of Lederer and Mills,[3] we calculate the effect of potential scattering in the host upon the additional T^2 contribution which results from the locally enhanced impurities.

II. METHOD AND RESULTS

A. General

To calculate the effect of potential scattering on the spin-fluctuation resistivity at low temperatures, we start with Mills and Lederer's[1] expression for the contribution to the resistivity that occurs when the conduction electrons scatter from spin fluctuations in the d band. This resistivity can be written in the following form[12]:

$$\rho = \frac{\rho_0}{k_B T} \int_0^\infty d\omega \int_0^\infty d\mathcal{E}_k \, f(\mathcal{E}_k)[1 - f(\mathcal{E}_k + \omega)] n(\omega) \times \frac{1}{k_F^4} \int_0^{2k_F} dq \, q^3 A(q,\omega) |F(q)|^2,$$

where $\mathcal{E}_k$ is the energy of the conduction electrons; q and ω are, respectively, the momentum and energy change (the units have been chosen such that $\hbar = 1$) that occurs when the conduction electrons are scattered via the s-d exchange interaction from the spin fluctuation; $A(q,\omega)$ is the spectral density function giving the momentum and energy distribution of the spin fluctuations; $n(\omega)$ is the Bose factor and is a measure of the excitation level of the fluctuation; $f(\mathcal{E}_k)$ is the Fermi-Dirac function; $F(q)$ is the form factor[7] associated with the Wannier functions for the d band; k_F is the Fermi wave vector of the conduction electrons; k_B is the Boltzmann constant; and ρ_0 is a parameter[12] which contains the density of states of the conduction electrons and the strength of the s-d interaction.

The temperature dependence at low temperatures is obtained by noting that as ω becomes larger than the thermal energy $k_B T$, the Bose factor goes to zero exponentially. As a result, the spectral density function need be considered only for values of ω which are $\lesssim k_B T$. In this region the spectral density function divided by ω is independent of ω, so the ω integration can be performed without any further knowledge of the functional form of the spectral density function. After integrating over ω and $\mathcal{E}_k$, one finds the low-temperature resistivity is given by

$$\rho = \left(\frac{\pi^2}{3} \rho_0 \frac{k_B^2}{k_F^4} \int_0^{2k_F} dq \, q^3 \frac{A(q,\omega)}{\omega} |F(q)|^2 \right) T^2, \quad T \to 0. \tag{1}$$

Note that the high-q end of the spectral density function is strongly weighted because of the q^3 factor in the integral.

For the case of a homogeneous system, the spectral density function is obtained directly from the imaginary part of the dynamic susceptibility $\chi(q,\omega)$ by using the relation

$$A(q,\omega) = 2\,\mathrm{Im}\chi(q,\omega). \tag{2}$$

In the following we will consider the spectral density function for both a uniformly exchange-enhanced system and a locally exchange-enhanced system.

B. Uniformly enhanced systems

To find the effect of potential scattering on the magnitude of the coefficient of the T^2 term which occurs in the spin-fluctuation resistivity of a uniformly exchange-enhanced system, one finds a dynamic susceptibility appropriate for the system and uses Eqs. (1) and (2) to evaluate the T^2 coefficient. A dynamic susceptibility for a uniformly exchange-enhanced system has been derived by Fulde and Luther[10] in their calculation of the effect of potential scattering on the specific heat. They calculated $\chi(q,\omega)$ in the presence of randomly distributed scattering centers each having a spherically symmetric potential. Their result is given by

$$\chi(q,\omega)=\frac{\chi_0(q,\omega)}{1-U\chi_0(q,\omega)}\,, \tag{3}$$

$$\chi_0(q,\omega)=N(E_F)\left(\frac{1+\frac{1}{2}(u+iu_0)\ln[(u+iu_0-1)/(u+iu_0+1)]}{1+\frac{1}{2}iu_0\ln[(u+iu_0-1)/(u+iu_0+1)]}\right), \tag{4}$$

where $u=(\omega/E_F)/(2q/q_F)$, $u_0=1/ql$, and l is the mean free path of the d-band electrons. Their result is valid for all values of l and for $(q/q_F)^2 \ll u \ll q/q_F$. Fulde and Luther's dynamic susceptibility cannot be used directly to calculate the T^2 coefficient in the spin-fluctuation resistivity because the q^3 weighting of the spectral density function in Eq. (1) (which did not occur in the specific-heat calculation) will almost certainly guarantee a substantial contribution from the region beyond which their result is valid.

In order to circumvent this problem, we have evolved an expression for the dynamic susceptibility which is expected to be valid for the entire range of q for a system with potential scattering. We did this by comparing Fulde and Luther's expression [Eq. (4)] with the well-known expression[11] for the dynamic susceptibility of an unenhanced system in which there is no potential scattering:

$$\begin{aligned}\mathrm{Re}\chi_0(q,\omega)&=N(E_F)\left(\frac{1}{2}+\frac{1-(u-v)^2}{8v}\ln\left|\frac{u-v-1}{u-v+1}\right|\right.\\&\qquad\left.-\frac{1-(u+v)^2}{8v}\ln\left|\frac{u+v-1}{u+v+1}\right|\right),\\\mathrm{Im}\chi_0(q,\omega)&=\pi N(E_F)\left(\frac{1-(u-v)^2}{8v}\,\Theta(1-(u-v)^2)\right.\\&\qquad\left.-\frac{1-(u+v)^2}{8v}\,\Theta(1-(u+v)^2)\right),\end{aligned} \tag{5}$$

where $v=q/2q_F$ and $\Theta(x)$ is the step function, which is equal to unity when the argument is positive and zero when the argument is negative. By noting that $\chi_0(q,\omega)$ given in Eq. (5) is valid for all q and ω for systems in which potential scattering can be neglected and by noting that Eq. (4) is valid for small q and ω for systems in which potential scattering cannot be neglected, we evolved the following interpolating expression for the dynamic susceptibility:

$$\chi_0(q,\omega)=N(E_F)\left(1+2u_0\frac{v^3}{1+v^6}\right)\times\left[\frac{\frac{1}{2}+g(u,u_0,v)+g(u,u_0,-v)}{1-iu_0\ln[(u+iu_0-1)/(u+iu_0+1)]}\right], \tag{6}$$

where

$$g(u,u_0,v)=\mathrm{Re}h(u,u_0,v)+i\Theta(\mathrm{Im}h(u,u_0,v))\,\mathrm{Im}h(u,u_0,v),$$

and

$$h(u,u_0,v)=\frac{1-(u+iu_0-v)^2}{8v}\ln\left(\frac{u+iu_0-v-1}{u+iu_0-v+1}\right).$$

Our confidence in Eq. (6) as a reasonable expression for $\chi_0(q,\omega)$ for a system with potential scattering is based on four aspects of its behavior: (i) It reduces to Eq. (4) in the range for which Eq. (4) is valid ($4v^2 \ll u \ll 2v$ and all values of l). (ii) It reduces to Eq. (5) in the range for which Eq. (5) is valid (all values of v and u and in the limit $l\rightarrow\infty$). (iii) It varies smoothly between the regions of validity of Eqs. (4) and (5). (iv) It is in good agreement with a result that was derived by deGennes.[13] His derivation of the dynamic susceptibility was for an unenhanced system with potential scattering but was for the special case of $\omega=0$. In comparing our interpolation for the case of $\omega=0$ with the results of deGennes we find that even for the case of a large amount of potential scattering ($lq_F=5$) the maximum difference is ~2% and, as the potential scattering is decreased, this difference becomes smaller and the two results both approach the static limit of Eq. (5).

We can now use the model to evaluate the effect of potential scattering on the spectral density function of a uniformly exchange-enhanced system [Eqs. (2), (3), and (6)]. In Fig. 1 we show $A(\bar{q},\bar{\omega})/N(E_F)$ (the spectral density function divided by the density of states at the Fermi level) for a range of $\bar{q}\equiv q/q_F$, for a fixed energy ratio of $\bar{\omega}=0.001$ ($\bar{\omega}\equiv\omega/E_F$), and for Stoner enhancement factor of 10.

The two solid curves which peak on the left show this spectral density function for two extreme cases: (i) there is no potential scattering ($l=\infty$) and (ii) the potential scattering is so large ($lq_F=5$) that the mean free path is close to an inter-

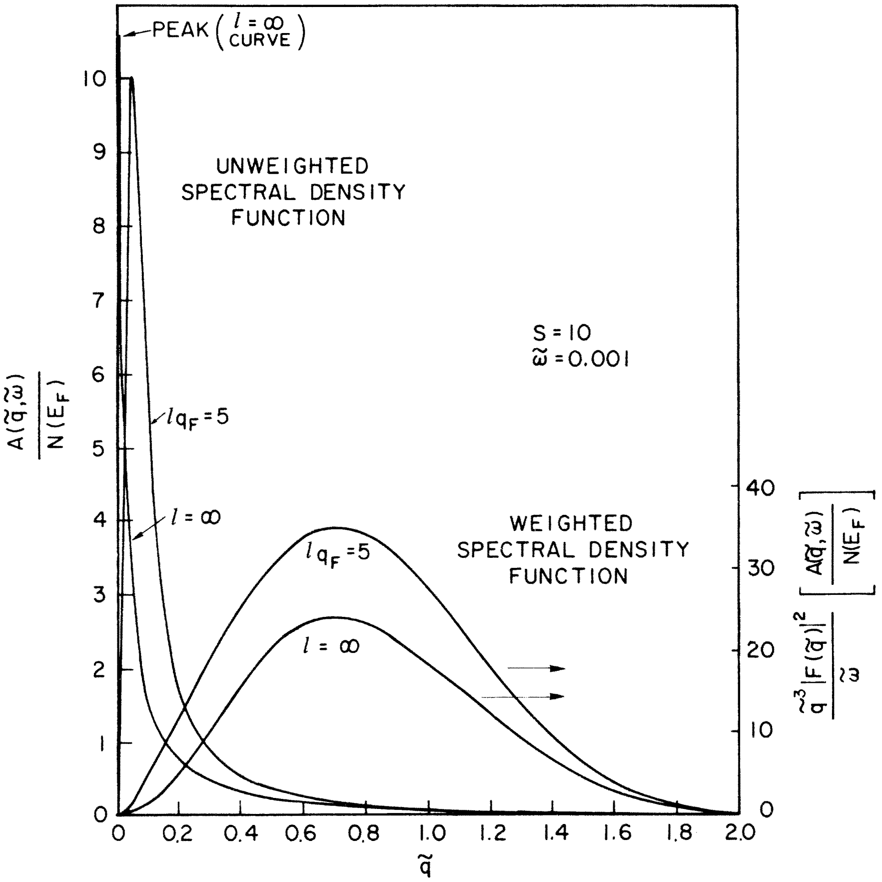

FIG. 1. Spectral density function $A(\tilde{q},\tilde{\omega})$ scaled by the density of states $N(E_F)$ is plotted as a function of the ratio $\tilde{q}$ of spin-fluctuation momentum to the Fermi momentum, for an energy ratio $\tilde{\omega}$ fixed at 0.001, and for a Stoner enhancement factor S of 10. The two solid curves which peak on the left show the spectral density function for the case of an infinite mean free path ($l=\infty$) and for the case of an extremely large amount of potential scattering ($lq_F=5$). The two solid curves which peak near the center show the weighted spectral density function for the same two cases. The form factor $F(q)$ has been approximated by using the Pd form factor of Ref. 14. The coefficient of the T^2 term in the spin-fluctuation resistivity is proportional to the integral over $\tilde{q}$ of the weighted spectral density function.

atomic spacing. As can be seen, the main effect of the potential scattering is to broaden and shift the peak of the spin-fluctuation distribution to a higher momentum.

The effect of potential scattering on the T^2 coefficient in the spin-fluctuation resistivity is found by inserting our spectral density function into Eq. (1). Because of the q^3 weighting of the spectral density function, the main contribution to the T^2 term comes from the tail of the spectral density function. This may be seen (in Fig. 1) by comparing the weighted spectral density function, $\tilde{q}^3|F(\tilde{q})|^2A(\tilde{q},\tilde{\omega})/\tilde{\omega}N(E_F)$, with the unweighted spectral density function. Since the T^2 coefficient is directly proportional to the integral over $\tilde{q}$ of the weighted spectral density function, the effect of potential scattering is found by evaluating this integral for various values of l and comparing the results. We present these results in terms of the fractional change in the T^2 coefficient, which is defined by

$$\frac{\Delta C_U}{C_U}=\frac{C_U(l)-C_U(\infty)}{C_U(\infty)},$$

where $C_U(l)$ is the T^2 coefficient of the uniformly exchange-enhanced system. In this calculation we have followed the work of Schriempf *et al.*[14] by taking $k_F=q_F/2$ and by using for $F(q)$ the approximation given by them for Pd. However, we note that the result is largely insensitive to the choices for $F(q)$ and k_F. [For example, if $F(q)$ is not allowed to fall off from unity at high q, the results shown will decrease by less than 6%. If k_F is doubled, the results will decrease by less than 8%. If $k_F \ll q_F$, a large increase over the results shown can occur, but in this case $C_U(l)$ will be orders of magnitude smaller and not of much interest.] Our results are shown by the lower curve in Fig. 2, where $\Delta C_U/C_U$ is plotted as a function of the mean-free-path parameter lq_F.

The result of the model calculation is to predict that in most cases the increase in the T^2 coefficient from the effect of potential scattering will be only a small fraction of the T^2 coefficient. For an alloy such as $Pd_{95}Rh_5$ (where the mean-free-path parameter lq_F is estimated to be between 100 and 200), the T^2 term is increased by only ~2%.

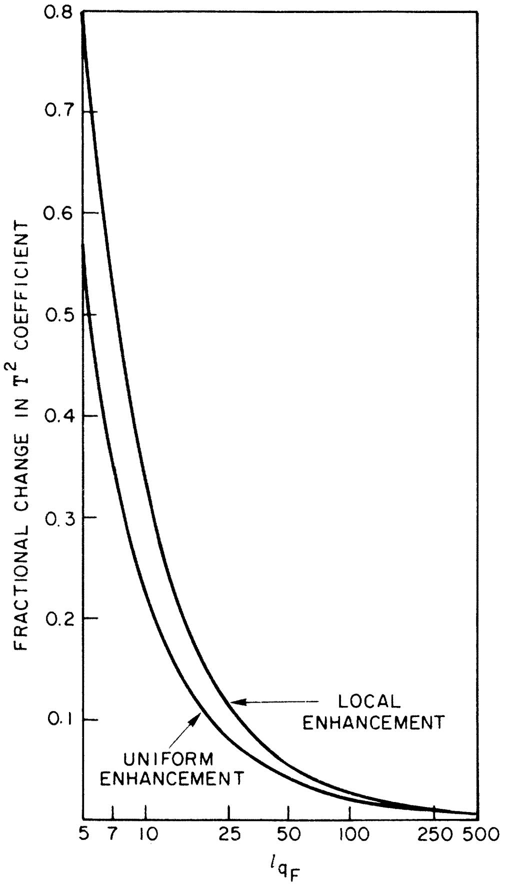

FIG. 2. Semilog plot of the fractional increase of the T^2 coefficient of the electrical resistivity as a function of the mean free path l of the d-band electrons. The lower curve shows this increase for a uniformly enhanced system with a Stoner enhancement factor of 10. In locally enhanced systems there is an additional T^2 term that results from the local enhancement. The upper curve shows the fractional increase in this T^2 coefficient as a function of the mean free path. For the case shown, the locally enhanced system is assumed to have a uniform background with a Stoner enhancement factor of 10.

C. Locally enhanced system

An analogous calculation can be made for a locally exchange-enhanced system. An example of such a system is an exchange-enhanced host containing an impurity which locally enhances the susceptibility around the impurity site, although not sufficiently to form a local moment. The local enhancement increases the spin fluctuations around the impurity site and, as a consequence of the conduction electrons scattering from these local spin fluctuations, an additional contribution to the T^2 term in the resistivity results. The spectral density function for such a system is given in the model of Lederer and Mills[3] as

$$A(q,\omega)=2\,\mathrm{Im}\chi(q,\omega)+2c\delta U\,\mathrm{Im}\left(\frac{\chi^2(q,\omega)}{1-\delta U\bar{\chi}(\omega)}\right),$$

where c is the impurity concentration; δU is the increase in the intra-atomic exchange interaction in the impurity cell; and $\bar{\chi}(\omega)$ is the average over q of the host susceptibility $\chi(q,\omega)$,

$$\bar{\chi}(\omega)=\frac{3}{Q_z^3}\int_0^{Q_z}dq\,q^2\chi(q,\omega),$$

where Q_z is the radius of the Brillouin-zone boundary (assumed spherical). The first term is just the spectral density function of the exchange-enhanced host, $A_U(q,\omega)$. The second term is then the contribution to the spectral density function from the localized spin fluctuations at the impurity sites, and we therefore write the spectral density function as

$$A(q,\omega)=A_U(q,\omega)+A_I(q,\omega).$$

For a large local enhancement and small ω the second term can be approximated[3] as

$$A_I(q,\omega)\approx 2c(\delta U\alpha)^2[\mathrm{Re}\chi(q,0)]^2\,\mathrm{Im}[\bar{\chi}(\omega)],$$

where $\alpha=[1-\delta U\,\mathrm{Re}\bar{\chi}(0)]^{-1}$ is the local-enhancement factor.

To find the T^2 coefficient for the locally enhanced system we proceed as in the uniform-enhancement case and evaluate Eq. (1). In this case, however, the spectral density function has the additional contribution $A_I(q,\omega)$, which will result in an additional contribution $C_I(l)$ to the T^2 coefficient. The dependence of $C_I(l)$ upon the mean free path of the host is a direct result of the fact that $A_I(q,\omega)$ is a function of the dynamic susceptibility of the host, which as we have seen is a function of l. We use the previously given results [Eqs. (3) and (6)] for $\chi(q,\omega)$ of the host and calculate the fractional increase of the impurity contribution to the T^2 coefficient;

$$\frac{\Delta C_I}{C_I}=\frac{C_I(l)-C_I(\infty)}{C_I(l)}.$$

The results of this calculation are shown by the upper curve in Fig. 2, where $\Delta C_I/C_I$ is plotted as a function of the mean-free-path parameter lq_F.

In this calculation we have assumed the entire change in the spectral density function from potential scattering is the result of the change in $\mathrm{Im}\bar{\chi}(\omega)$. This assumption will not be valid if the local-enhancement factor α is large, i.e., $\delta U\,\mathrm{Re}\bar{\chi}(0)\sim 1$. In this case, the small change that occurs in $\mathrm{Re}\bar{\chi}(0)$ as a result of potential scattering will significantly increase α. For this reason the upper curve of Fig. 2 should be viewed as a lower bound for the model.

Also, in this calculation we have taken $Q_z = 2q_F$, the Stoner enhancement factor $S = 10$, and have again used the form factor for Pd.[14] However, the results are largely insensitive to these choices. For example, $Q_z = q_F$ increases the result by less than 7%, $S = 20$ increases the result by less than 25%, and $F(q) = 1$ decreases the result by less than 25%.

III. CONCLUSIONS

It was pointed out in the Introduction that although the $Pd_{95}Rh_5$ system might be expected to act as a superenhanced Pd, measurements[4-6] of the T^2 term in the spin-fluctuation resistivity of the $(Pd_{95}Rh_5)_{1-x}Ni_x$ system did not show an enhancement over that of the $Pd_{1-x}Ni_x$ system. Since one of the major differences between the two systems is the large increase in potential scattering that results upon the addition of the Rh, it has generally been speculated that this scattering was affecting the spin fluctuations and causing a decrease in the spin-fluctuation resistivity at low temperatures. While potential scattering does indeed reduce the peak of the distribution of the spin fluctuations, the main effect of the potential scattering is to shift the distribution toward the high-q spin fluctuations. Since the increase in the high-q spin fluctuations has a stronger effect on the spin-fluctuation resistivity than the decrease in the low-q spin fluctuations, the net effect of the potential scattering on the spin-fluctuation distribution is, therefore, to increase the T^2 coefficients in both the uniform- and local-enhancement models. Our calculation predicts that the increase in the T^2 term in the spin-fluctuation resistivity of the $Pd_{95}Rh_5$ host will be ~2% as a result of the potential scattering and that the increase in the additional T^2 contribution which results from the addition of Ni to this host will also be ~2% as a result of the potential scattering in the host. Thus, the explanation of the unexpected values of the T^2 coefficients observed[4-6] in the $(Pd_{95}Rh_5)_{1-x}Ni_x$ system must reside in other mechanisms.

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