

Momentum-dependent electron self-energy in nearly ferromagnetic systems: Comparison of spin fluctuations and phonons

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The self-energy Σ is calculated in a two-parameter spin-fluctuation model. In contrast to the electron-phonon system, paramagnons have considerable spectral weight at large energies, $O(E_F)$, even very near the magnetic transition. The momentum dependence of Σ is important and leads to significant changes in the chemical potential and in the ratio m^*/m and to restoration of particle conservation, which is violated in the paramagnon model. The Eliashberg strong-coupling theory must be modified. Our results support resolution of the question of paramagnon model versus Fermi-liquid theory in favor of the latter.

I. INTRODUCTION

Since the early work of Doniach and Engelsberg¹ (DE) and Berk and Schrieffer^{2,3} (BS), the paramagnon model has been extensively applied to the calculation of normal state and superconducting properties of nearly ferromagnetic metals¹⁻⁶ and liquid ³He.⁷ Recent reviews have been given by Stamp⁸ and Béal-Monod.⁹ In this model the effective-mass enhancement is calculated from a one-paramagnon exchange approximation to the electron (or ³He atom) self-energy Σ . Although it was recognized at the start that a paramagnon is not a well-defined excitation, the analogy with phonons has been widely employed. In particular, it has always been assumed that the momentum dependence of Σ can be neglected and that, as the magnetic transition is approach, typical paramagnon energies ω_{SF} are much smaller than the Fermi energy E_F . We find that both of these assumptions are not valid: the paramagnons have considerable spectral weight at energies $O(E_F)$ even in strongly exchange-enhanced systems (Stoner factor $S \gg 1$) and, primarily because of this, the momentum dependence of Σ is important.

There have been some indications that paramagnons cannot be treated on the same footing as phonons. Layzer and Fay¹⁰ pointed out that the Σ calculated in the BS theory leads to a single-particle momentum distribution inconsistent with particle conservation. Missing vertex corrections were suggested as the cause. In related work Hertz *et al.*¹¹ showed that there is no Migdal's theorem for paramagnons.

We find that taking account of the momentum dependence of Σ restores particle conservation and we suggest that an "effective" Migdal's theorem may hold in a phenomenological interpretation of the theory. We also find, in contrast to the phonon case, that the change $\delta\mu$ in the chemical potential due to interactions is large (order E_F)

and that the "Migdal" sum rule, Eq. (7), used in the Eliashberg strong coupling theory^{3,12} does not hold. The momentum dependence of Σ right at the Fermi surface is however weak and thus, as for phonons, the relation $m^*/m \simeq 1 + \lambda$, with $\lambda = -\partial\Sigma/\partial\omega$, is a fairly good approximation. λ itself is reduced by the inclusion of the momentum dependence (about 25% in the case studied) thus tending to alleviate the problem that the paramagnon theory overestimates m^*/m .

II. SPIN FLUCTUATION AND PHONON CONTRIBUTIONS TO THE ELECTRON SELF-ENERGY

We consider a spin fluctuation (SF) contribution to the self-energy of the form

$$\Sigma(\mathbf{p}, \omega) = i \int \frac{d^4k}{(2\pi)^4} G(\mathbf{k}, \omega') t(\mathbf{p} - \mathbf{k}, \omega - \omega'), \quad (1)$$

where G is the single-particle Greens function and t is the particle-hole t matrix which, in the RPA-paramagnon theory (RPA: random-phase approximation), has the form

$$t(q, \omega) = I + \left(\frac{3}{2}\right) \frac{I^2 \chi_0(q, \omega)}{1 - I \chi_0(q, \omega)} \simeq \left(\frac{3}{2}\right) \frac{I^2 \chi_0}{1 - I \chi_0}. \quad (2)$$

Here I is the "contact" exchange interaction parameter and χ_0 is the susceptibility of the noninteracting system [$\chi_0(0, 0) = N(0)$]. The Stoner factor is then $S = [1 - N(0)I]^{-1}$ and the last form is valid for large S . For simplicity we assume zero temperature, uniform enhancement, and neglect all band-structure effects, i.e., essentially a model for liquid ³He.

In our actual calculation of Σ we employed a more general SF model in which $I \rightarrow I(q) = I/(1 + b^2 q^2)$.⁴

This is very similar to the potential⁷ and polarization potential^{7,13} models used by other authors. It has long been clear that the one parameter paramagnon model is inadequate for describing nearly ferromagnetic systems.⁸ A two-parameter momentum-dependent exchange interaction $I(q)$ was apparently first used by Schrieffer¹⁴ and Brinkman and Engelsberg.¹⁵ The effect of momentum dependence in the interaction has been discussed more recently by Ainsworth *et al.*¹⁶ and Coffey and Pethick.¹⁷ In the present work we are primarily interested in the effect of momentum dependence in the self-energy which has not previously been investigated. From now on we refer to the original one-parameter model^{1,2} as the "paramagnon" model and to the more general phenomenological models as "SF" models. Our results for Σ are thus not restricted to the paramagnon model. Later we discuss the validity of the RPA form, Eq. (2).

The strong-coupling treatment^{3,12} of Eq. (1) leads to

$$\text{Im}\Sigma(\varepsilon_p, \omega) = \left[\frac{k_F}{p} \right] \text{sgn}\omega \int_0^\omega d\omega' \int_{-E_F}^\infty d\varepsilon_k \text{Im}G(\varepsilon_k, \omega') \times F(\varepsilon_p, \varepsilon_k, \omega - \omega'), \quad (3)$$

where $p = |\mathbf{p}|$, $\varepsilon_p = p^2/2m - E_F$, and

$$F(\varepsilon_p, \varepsilon_k, \omega) = \frac{N(0)}{\pi} \int_{|p-k|}^{p+k} \frac{qdq}{2k_F^2} \text{Im}t(q, \omega). \quad (4)$$

$\text{Re}\Sigma$ can be obtained from a Kramers-Kronig dispersion relation. The p dependence of Σ occurs only in the prefactor in Eq. (3) and in the limits of Eq. (4). In the standard treatment one now follows Berk³ and argues that F is a weak function of p and k . This allows the replacement

$$F \rightarrow P(\omega) = \frac{N(0)}{\pi} \int_0^{2k_F} \frac{qdq}{2k_F^2} \text{Im}t(q, \omega). \quad (5)$$

$P(\omega)$ is the paramagnon spectral function used by a number of authors^{5,6} and corresponds to the $\alpha^2 F$ of the phonon case.⁶ For $\omega_{\text{SF}} \ll E_F$, we can set $p = k_F$ in the prefactor of Eq. (3) and Σ depends on ω only. As for phonons, $m^*/m = 1 + \lambda$ with

$$\lambda = 2 \int_0^\infty d\omega \frac{P(\omega)}{\omega}. \quad (6)$$

Equation (3) is now solved by employing a "sum rule" introduced by Migdal¹⁸ for the phonon case:

$$-\frac{1}{\pi} \int_{-E_F}^\infty d\varepsilon_k \text{Im}G(\varepsilon_k, \omega) \rightarrow -\frac{1}{\pi} \int_{-\infty}^\infty d\varepsilon_k \text{Im}G = 1. \quad (7)$$

This is equivalent to replacing $G \rightarrow G_0$ in Eq. (1) and should be valid to within corrections of order ω_{SF}/E_F . Equation (3) is thus reduced to a one dimensional integration.

In Fig. 1 we show the self-energy $\Sigma(\omega)$ that results for the SF-model parameters $N(0)I=0.95$ and $b=0.3/k_F$

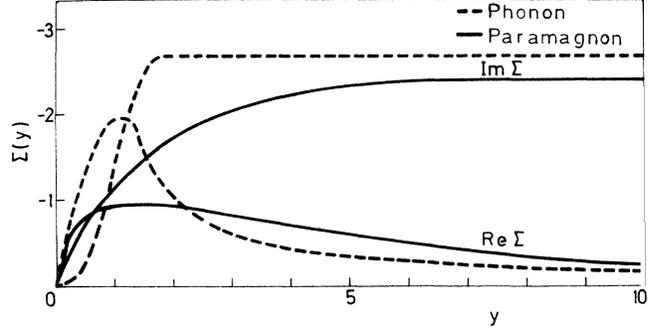


FIG. 1. Electron self-energy. Solid curves: $\text{Re}\Sigma/E_F$ and $\text{Im}\Sigma/E_F$ for the paramagnon case with parameters $N(0)I=0.95$ and $b=0.3/k_F$ (chosen so $\lambda=4.2$) with $y=\omega/E_F$. Dashed curves: $\text{Re}\Sigma/(2\omega_{\text{ph}})$ and $\text{Im}\Sigma/(2\omega_{\text{ph}})$ for the phonon case, $y=\omega/\omega_{\text{ph}}$.

which roughly corresponds to ³He near the melting pressure. $N(0)I$ is determined from $\chi(0,0)$ and b was chosen so $\lambda=4.2$. In this approximation Σ has the symmetries

$$\text{Im}\Sigma(-\omega) = \text{Im}\Sigma(\omega), \quad \text{Re}\Sigma(-\omega) = -\text{Re}\Sigma(\omega) \quad (8)$$

and thus $\text{Re}\Sigma(0) = \delta\mu = 0$. Also shown in Fig. 1 are the corresponding phonon curves calculated from a Lorentzian spectral function centered on $\omega = \omega_{\text{ph}}$ and adjusted to yield the same λ . Although the phonon and SF curves are quite similar, the important point is that Σ_{ph} is measured relative to ω_{ph} while Σ_{SF} is measured relative to E_F . The variation of Σ is confined to energies below several $\omega_{\text{ph}}(E_F)$ for the phonon (SF) case and the maximum magnitude is order ω_{ph} for phonons but order E_F for SF. Due to the size of ω_{SF} , extending the limit from $-E_F$ to $-\infty$ in Eq. (7) was actually not allowed for the SF case considered.

III. ELECTRON MOMENTUM DISTRIBUTION AND PARTICLE CONSERVATION

The electron momentum distribution $n(\varepsilon_p)$ is given by

$$n(\varepsilon_p) = \int_{-\infty}^0 A(\varepsilon_p, \omega) d\omega \quad (9)$$

where A is the electron spectral function given by

$$A(\varepsilon_p, \omega) = \frac{1}{\pi} \frac{|\text{Im}\Sigma|}{(\omega - \varepsilon_p - \text{Re}\Sigma)^2 + (\text{Im}\Sigma)^2}. \quad (10)$$

which satisfies the sum rule

$$\int_{-\infty}^\infty A(\varepsilon_p, \omega) d\omega = 1, \quad (11)$$

Eq. (11) is exact, in contrast to the "Migdal" sum rule, Eq. (7).

For the momentum-independent Σ , Eq. (11) is satisfied and with Eq. (8) it is easy to show that $n(\varepsilon_p)$ is symmetric about the line $n = \frac{1}{2}$:

$$n(-\varepsilon_p) = 1 - n(\varepsilon_p). \quad (12)$$

This can be seen in Fig. 2 where we show n for the cases of Fig. 1 with $\omega_{\text{ph}} = 0.01E_F$. The behavior of $n(\varepsilon_p)$ re-

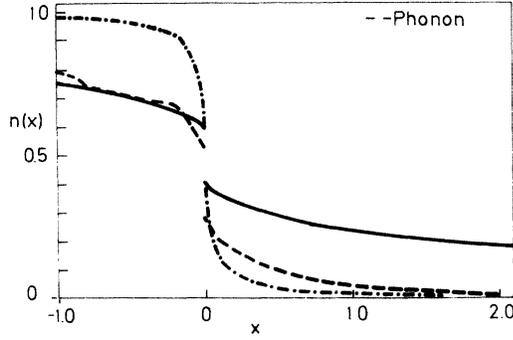


FIG. 2. Single-particle momentum distribution as function of $x = \varepsilon_p/E_F$ for the parameters $N(0)I=0.95$, $b=0.3k_F$ and, for the phonon case, $\omega_{ph}=0.01E_F$. Solid curves: Paramagnon model. Dashed curve: SF model with momentum-dependent Σ .

sulting from Eq. (12) shows that neglecting the p dependence of Σ necessarily leads to a violation of particle conservation. For the parabolic-band case, the particle number is

$$N = \frac{3}{2}N_0 \int_{-1}^{\infty} dx (x+1)^{1/2} n(x) \quad (13)$$

where $N_0 = (2mE_F)^{3/2}/(3\pi^2)$ is the particle number for the noninteracting system and $x = \varepsilon_p/E_F$. When $\Sigma = \Sigma(\omega)$, it follows that for $x \rightarrow \infty$, $n(x) \propto 1/x$ and N diverges. This does not cause concern in the phonon case because a *completely* momentum-independent Σ is not physical; momentum dependence on a scale of k_F is expected in any case and this will cause convergence of the integral in Eq. (13). Due to the smallness of ω_{ph}/E_F , however, such momentum dependence will have negligible effect on physically interesting quantities. The shape of $n_{ph}(\varepsilon_p)$, for example, will be essentially unaltered. For SF with $\omega_{SF}=0(E_F)$, this is not the case and the momentum dependence can be important.

Although it has been pointed out⁶ that “high-energy” paramagnons do not have to be treated on the same footing as phonons in strong-coupling superconductivity, it has always been assumed that for $S \gg 1$ the phonon analogy should be useful. We find that this is not the case. In Fig. 3 we plot $P(\omega)$ from Eq. (5) for several Stoner factors for the paramagnon model, $b=0$. The important point is that, although the peak moves to smaller ω as S increases, it *remains wide*. In Table I we compare several measures of ω_{SF} : The position of the peak ω_{peak} , the often used E_F/S , and the normalized first moment of $P(\omega)$, $\bar{\omega}_{SF}$, where we have cut the integrals off at $\omega = 1.5E_F$. It is seen that $\bar{\omega}_{SF}$ remains on the order of $E_F/2$ even for extremely large S and that E_F/S and ω_{peak} are not useful measures of typical SF energies. Thus the phonon analogy is for practical purposes *never* reasonable and the effect of momentum dependence and the large ω_{SF} must be investigated.

IV. NUMERICAL COMPUTATION OF $\Sigma(\varepsilon_p, \omega)$

We have numerically solved Eq. (3) with the $F(\varepsilon_p, \varepsilon_k, \omega)$ of Eq. (4). Since the replacement, Eq. (7), is

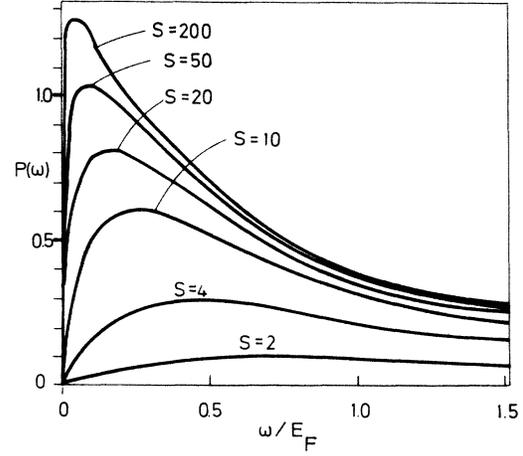


FIG. 3. Paramagnon spectral function defined by Eq. (5) for various Stoner factors.

not valid, Eq. (3) is now a nonlinear integral equation for $\text{Im}\Sigma(\varepsilon_p, \omega)$. $\text{Im}G$ can be expressed in terms of $\text{Re}\Sigma$ and $\text{Im}\Sigma$ through Eq. (10) with $\text{Im}G = -\pi A$. The general strategy is to use the momentum-independent results for Σ as input, compute $\text{Im}\Sigma$ from Eq. (3), $\text{Re}\Sigma$ from $\text{Im}\Sigma$ with a Kramers-Kronig dispersion relation and then use these results as input for the next iteration. We actually used as our starting approximation $\text{Im}\Sigma$ obtained by setting $\text{Im}G(\varepsilon_k, \omega') = -\pi\delta(\omega' - \varepsilon_k)$ in Eq. (3) which then reduces to an integral over the momentum-dependent spectral function $F(\varepsilon_p, \omega', \omega - \omega')$. In fact, a large part of the correction to $\Sigma(\omega)$ is already contained in this approximation; about 50% of the total correction to m^*/m , for example. We find good convergence after two or three further iterations.

The integrations were performed with Simpson’s rule with mesh sizes adjusted to give a maximum error in the final Σ of about 5%. The ε_k integration was particularly time consuming due to the complexity of the function F . This function is nonzero only for certain regions of ε_k which depend on ε_p and $\omega - \omega'$. A variable integration mesh size must be employed to insure inclusion of all contributions in a reasonable amount of computer time. We evaluated $\Sigma(\varepsilon_p, \omega)$ at 40 values of ε_p between $-E_F$ and $300E_F$ and at 70 values of ω between $-300E_F$ and $+300E_F$ with most of the points in the region of small

TABLE I. Typical definitions of paramagnon energy in units of E_F and λ from Eq. (6) for $b=0$.

S	E_F/S	ω_{peak}	$\bar{\omega}_{SF}$	λ
2	0.500	0.720	0.81	0.5
4	0.250	0.450	0.72	1.8
10	0.100	0.240	0.64	4.5
20	0.050	0.160	0.60	6.9
50	0.020	0.080	0.57	10.6
100	0.010	0.050	0.56	13.5
200	0.005	0.030	0.55	16.5
500	0.002	0.016	0.54	20.5
1000	0.001	0.008	0.54	23.6

ε_p and ω where Σ varies most rapidly. A linear interpolation was made between these points. The results were not sensitive to the way Σ was extrapolated to zero for large ε_p and ω .

We have not computed the special case of the range parameter $b=0$ because the δ -function approximation then yields an $\text{Im}\Sigma(\varepsilon_p, \omega)$ that increases linearly with ω for large ω . The calculation of $\text{Re}\Sigma$ is then more complicated; a twice-subtracted dispersion relation is necessary, for example. Although a linearly increasing ω dependence is apparently not forbidden on general grounds, the contact exchange interaction, $b=0$, is a rather unphysical approximation and we leave the study of the momentum dependence of this case to a future investigation.

Results for $\Sigma(\varepsilon_p=0, \omega)$ are shown in Fig. 4 for the same SF parameters as in Fig. 1. All curves approach zero as $\omega \rightarrow \pm\infty$. The symmetries, Eq. (8), no longer hold, $\delta\mu \approx 1.6E_F$ is large, and the exact sum rule, Eq. (11), is fulfilled. The momentum distribution, also shown in Fig. 2, now has a reasonable form for which Eq. (12) no longer holds, and the particle number is now conserved ($N=N_0$) to within about 2%.

As functions of p , $\text{Re}\Sigma$, and $\text{Im}\Sigma$ vary rather slowly for $0 < p < 2k_F$ and fall off fairly rapidly for $p > 2k_F$. Typical curves are shown in Fig. 5. For ω near zero and p near k_F , the ε_p variation of $\text{Re}\Sigma$ is slow: $\partial \text{Re}\Sigma / \partial \varepsilon_p \approx 0.07$. Thus the direct contribution of the p dependence to $m^*/m = (1+\lambda)/(1+\partial \text{Re}\Sigma / \partial \varepsilon_p)$ is small. However, λ is reduced from 4.2 to 3.2 by the inclusion of the momentum dependence yielding a overall reduction of m^*/m of about 25%.

We have not made a systematic study of the effect on the momentum dependence of Σ of varying the SF parameters I and b separately. The momentum dependence does not seem particularly sensitive to these parameters aside from the general diminishing of SF effects for decreasing I and increasing b which can be seen in Table I: for example, for $S=20$, the $b=0$ value $\lambda=6.9$ is reduced to $\lambda=4.2$ for $B=0.3/k_F$.

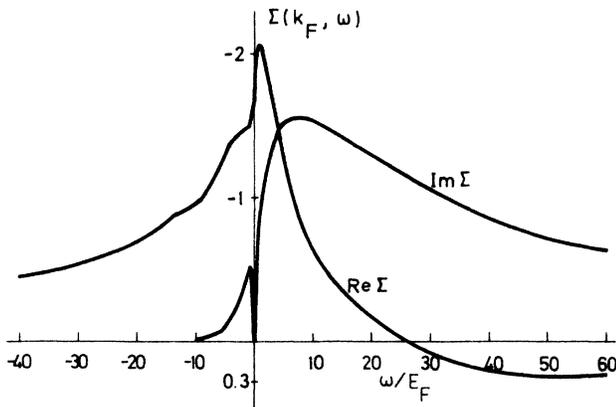


FIG. 4. Momentum-dependent self-energy as a function of energy computed from the nonlinear equations (3) and (4) for $N(0)I=0.95$ and $b=0.3/k_F$.

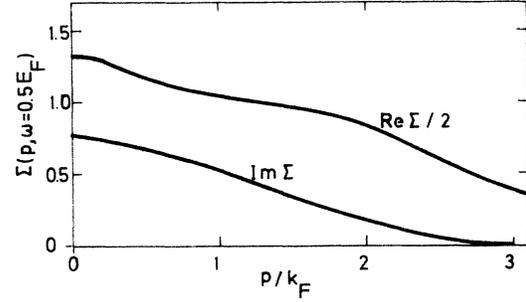


FIG. 5. Momentum-dependent self-energy as a function of momentum computed from the nonlinear equations (3) and (4) for $N(0)I=0.95$ and $b=0.3/k_F$.

V. CONNECTION WITH LANDAU THEORY

Our results shed some light on the long-standing controversy over the validity of the RPA susceptibility in Eq. (2). For $q=0$ and $\omega=0$, the paramagnon χ is given by

$$\chi_P(0,0)/\chi_0 = 1/[1 - N(0)I] \quad (14)$$

where $N(0)$ is the bare density of states. On the other hand, Landau theory yields the exact relation

$$\chi_L(0,0)/\chi_0 = (m^*/m)/(1 + F_0^a). \quad (15)$$

The difference in these two forms becomes important for finite q and ω : if the Landau form is extrapolated away from $q=\omega=0$ with the RPA-Lindhard function $\chi_0(q, \omega)$, the spin fluctuations are considerably weaker than in the paramagnon model. Unfortunately, the Landau theory does not tell us how to extrapolate Eq. (15) away from $q=0$. BS justified Eq. (14) by a rather convincing argument which, in light of our present results, appears to be incorrect. BS start with χ expressed through the exact particle-hole t matrix and replace the irreducible interaction with the constant I [or, more generally, $I(q, \omega)$]. This should not introduce factors of m^*/m and allows summation to

$$\chi(q, \omega) = \frac{Q(q, \omega)}{1 - I(q, \omega)Q(q, \omega)} \quad (16)$$

with

$$Q(q, \omega) = i \int \frac{d^4k}{(2\pi)^4} G(k, k_0) G(k+q, k_0+\omega). \quad (17)$$

A very simple argument^{3,19} now shows that $Q(0,0) = \chi_0(0,0) = N(0)$, if $\partial \Sigma / \partial p = 0$ and $\omega_{\text{SF}} \ll E_F$. Since neither of these conditions holds for SF, the BS argument fails. In fact, it has been shown²⁰ that relaxing the condition $\partial \Sigma / \partial p = 0$ leads to multiplicative renormalization of χ_0 . The BS argument does apply to the phonon case and shows that χ is not affected by phonons to leading order in ω_{ph}/E_F . It thus seems that Fermi liquid models, such as the polarization potential model,¹³ which reduce to $\chi_L(0,0)$ should be given preference.

VI. DISCUSSION

Concerning vertex corrections in the diagram for Σ , we point out a difference in the philosophy of the DE and BS approaches. DE start with a Hubbard-type Hamiltonian containing a parameter I_{DE} . The connection between I_{DE} and χ is not direct, i.e., the irreducible particle-hole interaction is a complicated function of I_{DE} . Vertex corrections are important¹¹ and can be included without double counting. This is not the case with BS who do not write down a Hamiltonian. Their I is a *phenomenological* parameter, essentially the $I(0,0)$ in Eq. (16), determined from the static, uniform susceptibility. It is thus very difficult to see what sort of vertex corrections could be added to the one SF exchange self-energy without double-counting contributions already effectively included in I .

The related fact that the paramagnon model is not consistent (conserving⁸) in the sense of Kadanoff and Baym is probably not particularly relevant in the phenomenological approach when one goes beyond the one-parameter model. Even in the paramagnon model of DE, the diagrams that must be added to make the theory consistent seem to be of the particle-particle ladder type that are not singular in the ferromagnetic limit.

We conclude that, although the phonon analogy is poor, an analog of Migdal's theorem may apply, nonethe-

less, and reasonable results can be obtained with the one SF exchange self-energy if account is taken of the momentum dependence and the large ω_{SF} and if a phenomenological SF propagator is used that reduces to the Landau $\chi_L(0,0)$. It should be emphasized that our results do not alter the basic SF-paramagnon concept, i.e., the importance of particle-hole diagram in nearly magnetic systems. Only the technical details and, to some extent, the interpretation are modified. In fact, we believe we have supplied some justification for the use of (suitably modified) SF theory.

SF models have recently been applied to heavy-fermion systems: the $T^3 \ln T$ term in the specific heat has been analyzed in terms of the paramagnon model²¹ and in terms of more general SF models.^{17,22} Several authors²³ have applied antiferromagnetic SF models to these systems. Improved calculations in this area should take into account the corrections discussed here, not only for the spin fluctuations but also for the phonon case since here $\omega_{ph} \gtrsim E_F \sim$ bandwidth.

Our modification of the Eliashberg strong coupling theory may also be important for the calculation of the superconducting transition temperature. In particular, since the effective SF energy is of the order of E_F , it is possible in principle that the paramagnon exchange mechanism could lead to much higher triplet transition temperatures than previously expected.

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