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MICROSCOPIC THEORY FOR THE FLUCTUATION-DRIVEN PHASE TRANSITION IN WEAK ITINERANT MAGNETS*

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ABSTRACT

The microscopic basis for a recent phenomenological theory for the thermodynamics near T_c of weak itinerant magnets is presented. Calculation of dynamic renormalization effects within paramagnon theory justifies the previous assumption of weakly temperature dependent Ginsburg-Landau α and β coefficients. The cutoff on the fluctuation phase space is found to go as $q_m \sim (T_c)^{1/3}$ rather than the usual inverse coherence length. In spite of the phase space reduction, as $T_c \to 0$, the phenomenological description becomes exact in a temperature region of order T_c. However, it is found that the α and β coefficients must be determined phenomenologically since no small parameter enters the calculation of their overall magnitude.

INTRODUCTION

Recent work[1,2] on spin fluctuations has explained why the random phase approximation for the Hubbard model $U \sum_i n_{i\uparrow} n_{i\downarrow}$ for a conduction band gives incorrect predictions for the experimental susceptibilities of extremely weak itinerant magnets. One faces the problem in deriving the Ginsburg-Landau functional

$$\mathcal{F} = \frac{1}{2} \sum_{q}^{q_m} |h_q|^2 (\alpha_F + \mu_F{}^2 q^2) + \frac{\beta_F \tilde{T}}{4!N} \sum_{\{q\}}^{q_m} h_q h_{q'} h_{q''} h_{-q-q'-q''} \quad (1)$$

where $\tilde{T} = TN(\epsilon_F)$ is the reduced temperature, h is a unit normalized field representing magnetization fluctuations, and the partition function $Z/Z_0 = \langle e^{-\mathcal{F}} \rangle$ is given as an ensemble average over the h fields.

The comparison with experiment fails if one assumes, as in the theory of superconductivity, that the order parameter susceptibility $\chi \propto \langle |h_0|^2 \rangle$ is given by α^{-1} calculated in the ladder approximation (RPA). The point is that $\alpha_{RPA} = 1 - 2UN(\epsilon_F)$ contains temperature dependence due only to the thermal average $\overline{N(\epsilon_F)}$ of the density of states. This results in the extremely weak dependence $\alpha_{RPA} = \alpha_{RPA}(T=0) + \mathcal{O}(\tilde{T}^2)$. Now in weak magnets χ^{-1} is observed to have linear[3] rather than quadratic dependence on T over several T_c. Further the Curie coefficient obtained by expanding α_{RPA} around its zero is proportional to ϵ_F/T_c, whereas experimentally this number should be more like unity.

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The suggestion of Murata and Doniach[1] (hereafter called I) is that the leading temperature dependence in χ^{-1} may come from the β_F term. With the Hartree factorization

$$\sum_{\{q\}} h^4 \approx 6 \sum_{qq'} |h_q|^2 < |h_{q'}|^2 > -3 \sum_{qq'} < |h_q|^2 > < |h_{q'}|^2 >$$

of the β_F term, the model is solvable, and we obtain

$$\chi_q^{-1} \sim D_q \equiv < |h_q|^2 > = (\alpha_F + \beta_F T\xi/2 + \mu_F^2 q^2)^{-1}$$

with $\xi = N^{-1} \sum_{q < q_m} D_q$. Not too close to T_c, ξ is roughly $\xi_0 = \Omega_a q_m / 2\pi^2 \mu_F^2$, with Ω_a the atomic volume. The β_F term can thus provide the required Curie temperature dependence in χ provided q_m is sufficiently large.

The magnitude of q_m is not given, as one might expect, by the inverse of the finite or zero temperature coherence length. Rather, it is argued below that the momentum sum defining ξ encompasses the thermal modes. If these modes are assumed to be overdamped paramagnons with width $\Gamma(q) \sim q^3$, one immediately obtains $q_m \sim \tilde{T}^{1/3}$, a result obtained from less obvious means below. The anomalously large q_m and partial success of the fluctuation model is thus due to the extremely "shallow" q^3 paramagnon dispersion.

LOWEST ORDER DYNAMIC COUPLING

The free energy (1) does not omit the finite (Matsubara) frequency modes. These have been integrated out and because of coupling effects renormalize α_F and β_F. To lowest order in this coupling the dynamic susceptibility is given by

$$D_q(\omega \pm i\delta) = [\eta + \mu_F^2 q^2 \mp i\omega/\gamma q]$$

where $\eta = \alpha_0 + \alpha^{(1)} + \beta_0 \tilde{T}\xi/2$, $\gamma = 2V_F/(2\pi\, UN(\epsilon_F))$, and α_0 and β_0 are nominal values given by $\alpha N(\epsilon_F)$ and $\beta N(\epsilon_F)$ in the notation of I. Here $\alpha^{(1)}$ is a functional of $D_{qn} = D_q(\omega_n)$ and the electron Green's function $G_{kn} = [\omega_n - \epsilon_k]^{-1}$, where ω_m is the Matsubara frequency:

$$\alpha^{(1)} = \frac{2U^2T^2}{N^2} \sum_{kqnm} D_{qm}\left[2G_{k-q,n-m}\, G^3_{kn} + G^2_{k-q,n-m}\, G^2_{k,n}\right]$$

The primed sum implies for m=0, only values of $q > q_m$ are taken; the rest are included in ξ. The q_m is determined variationally.

Converting the Matsubara sums in the standard fashion to integrals in the complex plane, we deal with terms in the temperature derivative of $\alpha^{(1)}$ as follows: 1) The derivative with respect to explicit Fermi factors generates terms of order $\tilde{T}$ and $\tilde{T}\ln\tilde{T}$. 2) The term containing the boson factor $n(\omega)$ can be written, after some manipulation, as:

$$\alpha^{(1)}_{\mathrm{Boson}} = - \frac{U^2 N''(\epsilon_F)}{N} \left\{ \frac{1}{\pi} \sum_q \int d\omega' \left[n(\omega) - \frac{T}{\omega'} - \frac{1}{2} \right] \mathrm{Im} D_q(\omega + i\delta) + T \sum_{q > q_m} \mathrm{Re} D_q(0) \right\} \tag{2}$$

The cutoff q_m is determined by requiring that $\left[\frac{\partial}{\partial T} + \frac{\partial q_m}{\partial T}\frac{\partial}{\partial q_m}\right]\alpha^{(1)}_{\mathrm{Boson}}$ vanish. As shown below, this condition reduces to $q_m \sim T^{1/3}$.[3] The implicit dependence on η generates a term $\frac{\partial \alpha^{(1)}}{\partial \eta}\frac{\partial \eta}{\partial T}$. The explicit form for $\frac{\partial \alpha^{(1)}}{\partial \eta} \approx \left.\frac{\partial \alpha^{(1)}}{\partial \eta}\right|_{\eta=0} < 0$ is found to be

$$\frac{d\alpha^{(1)}}{d\eta} = \frac{U^2 N''(\epsilon_F)}{N} \left[\sum_q (\gamma q)^2/\pi\Gamma(q) + \sum_q \gamma^2 q \ln\left(\frac{qV_F}{\Gamma(q)}\right) \right] \tag{3}$$

where $\Gamma(q) = \gamma q(\eta + u_F{}^2 q^2)$. We see that (3) is approximately constant and of order unity. Thus

$$\frac{d}{dT}\eta \approx \frac{d}{dT}(\alpha_0 + \beta_0 \tilde{T}\xi/2) + \left.\frac{\partial \alpha^{(1)}}{\partial \eta}\right|_{\eta=0} \frac{d}{dT}\eta + \mathcal{O}(\tilde{T}\ln\tilde{T}) .$$

Integrating this and defining $\eta = \alpha_F + \beta_F \tilde{T}\xi/2$, we find to order $\tilde{T}^2 \ln \tilde{T}$:

$$\alpha_F = (\alpha_0 + \alpha_0{}^{(1)})/(1 - \left.\frac{\partial \alpha^{(1)}}{\partial \eta}\right|_{\eta=0})$$

$$\beta_F = \beta_0/(1 - \left.\frac{\partial \alpha^{(1)}}{\partial \eta}\right|_{\eta=0}) \tag{4}$$

Here $\alpha_0{}^{(1)}$, which is also found to be of order one, is $\alpha^{(1)}$, evaluated for $\eta=0$ and $T=T_c$. Equation (4) shows the qualitative way the dynamic renormalization effects enter. Comparable corrections are expected from higher order couplings since $UN(\epsilon_F) \sim 1$ appears to be the relevant parameter.

DETERMINATION OF q_m

This is rather delicate. Writing

$\mathrm{Im}D_q(\omega+i\delta) = (\gamma q/2)d\ln(\Gamma^2(q)+\omega^2)/d\omega$, we integrate (2) by parts. We next split up the weight of

$$\frac{1}{\pi}\ \frac{\partial}{\partial\omega}\,[n(\omega)-T/\omega-1/2] = \frac{T/\pi}{\omega^2+T^2} + \frac{1-\pi}{\pi\omega}\ g(\tfrac{\omega}{T}) \tag{5}$$

into a Lorentzian part and a function g of unit weight and asymptotic behavior $g(x)/x \to x^{-4}$. Substituting (5) and forming the derivative $[\frac{\partial}{\partial T} + \frac{dq_m}{dT}\frac{\partial}{\partial q_m}]$, we obtain a sum of terms proportional to

$$\int_0^{2k_F}\frac{dq\gamma q^2}{\Gamma(q)+T} + \frac{1-\pi}{\pi}\int_0^{2k_F} dq\gamma q\int\frac{dx}{x^2}\ \frac{xg(x)T}{\Gamma^2(q)+x^2T^2}$$

$$+ T\,\frac{q_m^2}{\eta+\mu_F^2 q_m^2}\ \frac{dq_m}{dT} - \int_{q_m}^{2k_F}\frac{q^2dq}{\eta+\mu_F^2 q^2} \tag{6}$$

In (6) one may set $\eta=0$ to good approximation. One then obtains a sum of the form $aq_m+bT^{1/3}+cT\,dq_m/dT$, which has the solution $q_m\sim T^{1/3}$. The coefficient can be obtained numerically from (6) if necessary.[4]

DISCUSSION

It was assumed in I that the temperature dependence of α_F and β_F is relatively weak. The above suggests fairly weak $T^2\ln T$ dependence, with a coefficient which presumably cannot be readily calculated. However, at some point for sufficiently low T_c, we expect the $T^{4/3}$ dependence from $\beta_F T\xi$ to dominate and the model (1) to become appropriate.

Criteria for the validity of the Hartree approximation to (1) are given in I in terms of the two small parameters T/T_0 and $\epsilon \sim T^2/(T-T_c)\cdot T_0$. Since $T_0 \sim q_m$, the Hartree theory becomes valid at sufficiently low T_c over a range determined essentially by the constancy of α_F and β_F. This is presumably $|T-T_c|/T \sim \mathcal{O}(1)$.

As mentioned in I, Sc_3In with $T_c \sim 6K$ fits the model, whereas $ZrZn_2$ with $T_c \sim 25K$ does not. Systems with considerably lower T_c's are presumably required for extremely good fits to the Hartree theory. However, in the event such systems are found, one may be able to test for the $T^{1/3}$ dependence by including a temperature-dependent q_m in the Hartree theory.

Unfortunately the above results seem to indicate that contrary to the suggestion of Moriya and Kawabata[2] a proper calculation of α_F and β_F from given bandstructure is not feasible because the expansion parameter $UN(\epsilon_F)$ is not small.

Full details of the calculation will be published elsewhere.

REFERENCES

1. K.K. Murata and S. Doniach, Phys. Rev. Letters 29, 285 (1972)
2. T. Moriya and A. Kawabata, J. Phys. Soc. Japan 34, 639 (1973) and Technical Report of the Institute for Solid State Physics, University of Tokyo, Series A, No. 574 (1973).
3. See, for example, the experimental references in Ref. 1.
4. The crossover behavior in the numerical work of Moriya and Kawabata indicates that q_m can be of order k_F even for $T/\epsilon_F \sim 0.01$.