Correlation Theory of Planar Magnets for $T \geqslant T_c$

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A self-consistent theory for static and dynamic properties of planar magnets including quantum and correlation effects is presented. The renormalization and damping of the potentially soft mode is calculated. A central peak absorbing the spectral weight near the transition temperature is found. Qualitative agreement is obtained with observations made on Pr, which approximately represents a singlet-doublet model. The correlation theory is a systematic generalization of the random-phase approximation with an equally wide range of applicability.

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Planar magnets constitute a class of systems with a wide range of interesting physics very different from the isotropic Heisenberg magnets. This is a consequence of the competition between the planar anisotropy (D), which favors the nonmagnetic singlet ground state, and the exchange interaction (J_0) which favors alignment of spins in the plane. The outcome depends on the lattice dimension (d) with substantial implications for the phase diagram. As the ordering temperature (T_c) or the critical ratio ($R = D/2J_0$) is approached from above, differently oriented ordered clusters are building up on the background of the singlet ground-state matrix. The conventional exciton theory in the random-phase approximation (RPA)[1] is considering the creation of independent spins in the matrix and is therefore not capable of describing the short-range correlation. We will here show that the correlation effects in a simple way can be included using the correlation theory, which was successfully applied to the Heisenberg magnets EuO and EuS for $T > T_c$.[2] The theory represents a systematic generalization of the RPA theory for several dynamical variables (here two) and has as such a much wider applicability than presently discussed. The inclusion of correlations has two important effects for the transverse susceptibility $\chi^{xx}(q,\omega)$: firstly giving damping and renormalization of the RPA excitonic modes and secondly producing a central peak (CP) representing spin diffusion of the correlated regions. This holds for both the singlet-singlet and singlet-doublet models for which the RPA only gives the excitonic mode. However, a low-frequency response was observed in Pr,[3] which had a broad maximum as a function of wave vector at the minimum of the exciton branch. The intensity varies with temperature and pressure.[4] It has not previously been satisfactorily explained. Pr at zero pressure is well approximated by the singlet-doublet model[5] and it is suggested that the observed CP largely is due to the presently discussed correlation effect. This was not included in previous theoretical treatments of planar magnets.[6] Using a Landau functional approach for the related transverse Ising model, Klenin and Hertz[7] found evidence for a CP, but they were forced to make severe approximations which prevented realistic results to be obtained. There are several planar magnets representing different lattice dimensions and ratios, for example, Pr ($d = 3$, $R = 0.93$),[3,4] $RbCrCl_4$ ($d = 2$, $R = 0.005$),[8] $CsFeCl_3$ ($d = 1$, $R = 1.07$).[9] Pr has a nearly critical ratio and is presumably therefore the only material in which both the excitonic and a central mode have so far been observed. However, the ratio R may be varied by application of external pressure or field and the present theoretical predictions may be tested in other, perhaps more ideal singlet-doublet (or singlet-singlet) systems, for example, $CsFeCl_3$.

The planar magnets are described by the Hamiltonian

$$H = -\tfrac{1}{2}\sum_q J_q \vec{S}_q \cdot \vec{S}_{-q} + D\sum_q S_q^{z\,2}. \qquad (1)$$

The exchange interaction J_q equals $J_0\gamma_q$ and for nearest-neighbor interaction $\gamma_q = \sum_R \exp(iqR)/\rho$, where ρ is the number of neighbors. For $D > 0$ and an effective $S = 1$ the single-ion ground state $|1\rangle$ is a singlet with a doublet $|2\rangle$ and $|3\rangle$ at the energy D. With standard basis operators $a_{pn} = |p\rangle\langle n|$ for calculating the dynamical response function $\chi^{\alpha\alpha}(q,\omega)$ one can show that $\chi^{xx}(q,\omega)$ and $\chi^{zz}(q,\omega)$ are uncoupled in zero magnetic field. However, $S_q^{\,x} = a_{12}^{\,q} + a_{21}^{\,q}$ is coupled to the quadrupolar-type operator $L_q^{\,x} = (S^yS^z + S^zS^y)_q = i(a_{12}^{\,q} - a_{21}^{\,q})$. The corresponding response function may be measured by sound-wave measurements; it must be included in the calculation of $\chi^{xx}(q,\omega)$, which can be measured by neutron scattering. The formal solution to the problem for two operators S and L considered as a vector A was given by Mori[10]:

$$(A|A^\dagger)_z = \chi[z - i\langle\omega\rangle + \Phi(z)(\langle\omega^2\rangle - \langle\omega\rangle^2)]^{-1}, \qquad (2)$$

where

$$(A|B)_z = \int_0^\infty dt\, e^{-zt} \int_0^\beta d\lambda \{\langle A(t - i\lambda)B\rangle - \langle A\rangle\langle B\rangle\},$$

$\beta = 1/k_B T$ and χ is the static susceptibility matrix. The moment matrices $\langle\omega\rangle$ and $\langle\omega^2\rangle$, the correlation matrix $\langle AA^\dagger\rangle$, and the dynamical response matrix $\chi(q,\omega)$ can be self-consistently calculated by exact relations from (2).

The essential problem is to find an approximate solution for the random-force relaxation matrix $\varphi(z)$. It was recently found for the case of one dynamical variable S_q^z that a two-pole approximation[2] for $\chi^{zz}(q,\omega)$ $(\omega = \pm\Omega + i\Gamma)$ yields an exhaustive and accurate description for static and dynamic properties for $T > 1.02T_c$ for the Heisenberg magnets EuO and EuS. It corresponds to including d^2/dt^2 in the Ginzburg-Landau equation, which has been used extensively in the problem of structural phase transitions.[10] In the present theory it corresponds to the assumption of a Lorentzian decay in the frequency range of interest for the random force, or $\varphi(z) = (z + 2\Gamma)^{-1}$, where Γ is calculated self-consistently by a mode-mode decoupling of $\varphi(z)$. The same approach can be used here for $\chi^{zz}(q,\omega)$. However, for planar magnets it is $\chi^{xx}(q,\omega)$ which is of most interest. With two dynamical variables the analogous approximation is $\varphi_{11}(z) = (z + 2K_1)^{-1}$ and $\varphi_{22}(z) = (z + 2K_2)^{-1}$. If we simplify further by introducing only one parameter $K_q = K_1 \sim K_2$, it turns out that K_q can be determined without decouplings approximately from the exact $\langle\omega_q^2\rangle^{xx}$ in this case. Because of the matrix nature of the problem (2) there are four complex poles $(\pm\Omega_q, i\Gamma_q)$ and $(\pm\epsilon_q, i\delta_q)$ in two groups for $\chi^{xx}(q,\omega)$. When the groups are separate the spectrum (2) for $\chi^{xx}(q,\omega)$ is well approximated by a weighted sum of two normalized two-pole functions,

$$\chi^{xx}(q,\omega) = \chi_q^{xx}\frac{2}{\pi}\left\{(1-P)\frac{\Gamma_q(\Omega_q^2+\Gamma_q^2)}{(\omega^2-\Omega_q^2-\Gamma_q^2)^2+4\omega^2\Gamma_q^2} + P\frac{\delta_q(\epsilon_q^2+\delta_q^2)}{(\omega^2-\epsilon_q^2-\delta_q^2)^2+4\omega^2\delta_q^2}\right\}. \qquad (3)$$

In terms of the RPA frequency $\omega_q = \{D(D - J_q Q)\}^{1/2}$ and the matrix elements Δ_{11}^2 and Δ_{22}^2 of $\langle\omega^2\rangle - \langle\omega\rangle^2$ one finds, when Δ_{11}^2 and K_q are small, the following simple expressions for the parameters in (3):

$$\Omega_q = \{\omega_q^2 + \Delta_{22}^2\}^{1/2},\quad \epsilon_q = 0,\quad P = \Delta_{22}^2/\Omega_q^2,\quad \Gamma_q = K_q P,\quad \delta_q = 2K_q(1 - P/2),\quad K_q^2 = \Delta_{11}^2/P. \qquad (4)$$

The excess second moments, which give the deviation from the RPA result, are given exactly by

$$\Delta_{11}^2 = (J_0 - J_q)\chi_q^{xx\,-1}N^{-1}\sum_k \gamma_k\{\langle S_k^y S_{-k}^y\rangle + \langle S_k^z S_{-k}^z\rangle\},$$
$$\Delta_{22}^2 = J_0 D Q^{-1} N^{-1}\sum_k \gamma_k\{4\langle S_k^x S_{-k}^x\rangle + \langle S_k^y S_{-k}^y\rangle - \langle L_{k-q}^y L_{q-k}^y\rangle + \langle S_k^z S_{-k}^z\rangle - \langle L_{k-q}^z L_{q-k}^z\rangle\}. \qquad (5)$$

By inspection we notice that $\Delta_{11}^2 \to 0$ for $q \to 0$ and at T_c when $\chi_{q_0}^{xx} \to \infty$ at the ordering vector q_0; on the other hand Δ_{22}^2 is large in particular near T_c and is essentially proportional to ratio of the correlations $\langle S_0^x S_R^x\rangle/\langle S_0^x S_0^x\rangle$ on different and on the same site, since[5] $Q = 2(\langle S_x^2\rangle - \langle S_z^2\rangle)$. At the transition temperature T_c the RPA frequency $\omega_{q_0} \to 0$. However, the coupling between S_q^x and L_q^x completely changes the dynamical behavior relative to the picture obtained by the RPA approximation. The excitonic mode at Ω_q does not go soft, but loses all its spectral weight to the central peak at T_c, since $\Omega_q^2 \to \Delta_{22}^2$ and $P \to 1$. For large temperatures Δ_{11}^2 approaches $4J_0^2(1-\gamma_q)/3\rho$, i.e., the second moment for the pure Heisenberg system. For $D \to 0$ the coupling between S_q^x and L_q^x vanishes and the theory reduces to that used for EuO.[2]

The physical interpretation of the result is that correlated clusters of spins in the plane are building up near T_c in the singlet ground-state matrix. The dynamical behavior of these gives a central peak. The half-width of that is found to be proportional to q^2 at T_c indicating diffusional behavior. The width of the central peak vanishes

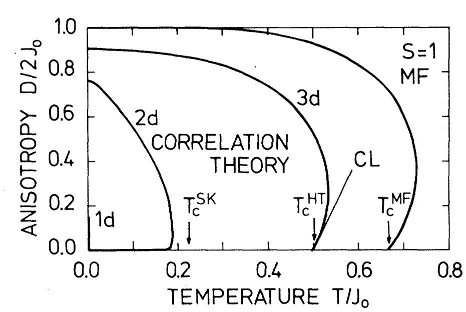

FIG. 1. The calculated (Ref. 11) transition temperatures T_c as a function of $D/2J_0$ for $d=3$ and 1 compared with the mean-field theory (MF) and the classical approximation $\langle SS\rangle = kT\chi$. The high-temperature-expansion T_c for $d=3$ and 2 are indicated by T_c^{HT} and T_c^{SK}.

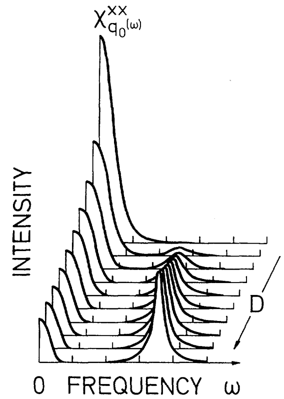

FIG. 2. The calculated $\chi^{xx}(q_0, \omega)$ for $d=3$ showing a central peak and an excitonic mode as a function of decreasing $\omega_{q_0} = [D(D-J_{q_0}Q)]^{1/2}$ for equidistant values of D. The foremost spectrum is calculated for parameters corresponding to Pr at $T=5$ K. All spectra are normalized to the same area.

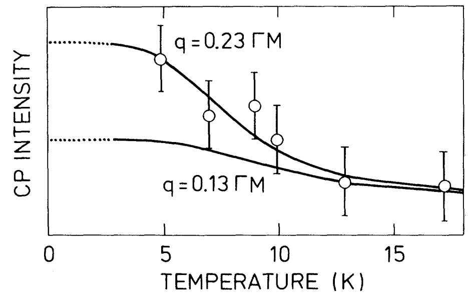

FIG. 3. Calculated temperature and wave-vector dependence of the central peak in Pr compared with polarized-neutron scattering measurements for $q=0.22\Gamma M$ by Burke *et al.* (Ref. 4). At low temperatures the singlet-doublet model is not applicable to Pr because of other effects.

at T_c indicating normal critical slowing down. A qualitatively similar, but less explicit, result is emerging from the Landau functional approach, in which the central peak can be understood as coming from $\chi^{zz}(q,\omega)$, which is locally coupled to $\chi^{xx}(q,\omega)$ by the local molecular field in the correlated regions. However, because of too severe approximations Klenin and Hertz[7] underestimate the weight of the CP by neglecting the dispersion effects.

The introduction of the pair correlation effects in the renormalization factors Q, Δ_{11}^2, and Δ_{22}^2 yields clearly a dependence on the lattice dimensionality.

Self-consistent numerical calculations[11] were performed for $d=3$ fcc, $d=2$ square, and $d=1$ lattices. The phase diagram is shown in Fig. 1 as a function of the ratio $R=D/2J_0$. For $d=3$ there is no order above the critical ratio $R_{\text{fcc}}^{(3)}=0.901$. This may be compared with the high-temperature series expansion (HTE), $R_{\text{fcc}}=0.858$.[12] For $D=0$ one finds $T_c^{(3)}=0.499$ in agreement with HTE.[13] T_c increases initially with increasing D as expected on the basis of the classical relation $\langle SS\rangle = kT\chi$, which is used in the classical soliton theories. However, this relation is inadequate for large D where quantum effects are dominant and use must be made of the exact relations. For $d=2$ the critical ratio is $R_{\text{sq}}^{(2)}=0.763$. For a triangular lattice the HTE gives $R_{\text{tr}}=0.710$.[12] It is interesting that over an infinitesimal range of $D \gtrsim 0$, $T_c^{(2)}$ rises from 0 to a temperature close to that discussed by Stanley and Kaplan,[13] T_c^{SK}. Thus a very small planar anisotropy causes the two-dimensional Heisenberg magnets to order at rather high temperatures, as seen experimentally.[8] For $d=1$ the system is infinitely susceptible to order at infinitesimal temperatures up to $R^{(1)}=0.11$. Figure 2 shows the calculated dynamical behavior (2) of the normalized $\chi^{xx}(q_0,\omega)$ for $d=3$ at a fixed wave vector q_0. The parameters D and J_q (anisotropic) used for the foremost curve are chosen to represent the measured exciton mode for Pr at $T=5$ K, and $q_0=0.23\Gamma M$ is the minimum of the dispersion relation. The effect is shown when ω_q is decreased by decreasing D equidistantly; a temperature change has similar effect because of the temperature dependence of Q. The increasing damping and decreasing intensity of the excitonic mode and the simultaneous increase of the central peak are evident; at T_c the latter becomes a δ function. This behavior is typical for the $S=1$ planar magnet. A central peak was observed[3,4] in Pr and the temperature and wave-vector dependence of the intensity is in agreement with the predicted behavior[3,4] $\sim \chi_q^{xx}\Delta_{22}^2/\Omega_q^2$, which approximately behaves like the soft-mode frequency to the power -4. A comparison is shown on Fig. 3. In reality Pr is more complicated than the singlet-doublet model; the effect of the higher levels and possible couplings to nuclear spins must be included. Therefore, additional features occur at low temperatures and under pressure, which cannot be accounted for by the singlet-doublet model. A detailed analysis will be published elsewhere.

In summary, the described correlation theory makes use of exact sum rules to calculate self-consistently static and dynamic properties on a basis of a realistic assumption of the line shape of the response function. It accounts for the phenomena observed in systems with a potentially soft mode. RPA and classical theories are very inaccurate for such systems. Because of the simple and general nature of the approximation scheme in the correlation theory it may be considered as a generalization of the RPA with a wide range for applications.

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Scaling Theory of Interacting Disordered Fermions

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A scaling theory for the interacting disordered fermion problem is constructed by extending the perturbation in coupling constant to second order. A scaling hypothesis produces a set of scaling equations which incorporates both localization and interaction. The resulting exponents are compared with experiments and further experimental tests of the theory are proposed.

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Many disordered electronic systems undergo a metal-to-insulator transition as the amount of disorder is increased. In the past few years, increasing evidence has accumulated that the nature of the transition is governed by two aspects of the problems: (i) Anderson localization, i.e., the behavior of a single-electron wave function in the presence of a random potential and (ii) the interaction among electrons in the presence of disorder. By now, a scaling theory of the Anderson-