Quantum frustrated and correlated electron systems

P Thalmeier
Max Planck Institute for Chemical Physics of Solids, 01187 Dresden, Germany

Abstract
Quantum phases and fluctuations in correlated electron systems with frustration and competing interactions are reviewed. In the localized moment case the $S=1/2 J_1 - J_2$ model on a square lattice exhibits a rich phase diagram with magnetic as well as exotic hidden order phases due to the interplay of frustration and quantum fluctuations. Their signature in magnetocaloric quantities and the high field magnetization are surveyed. The possible quantum phase transitions are discussed and applied to layered vanadium oxides.

In itinerant electron systems frustration is an emergent property caused by electron correlations. It leads to enhanced spin fluctuations in a very large region of momentum space and therefore may cause heavy fermion type low temperature anomalies as in the 3d spinel compound LiV$_2$O$_4$. Competing on-site and inter-site electronic interactions in Kondo compounds are responsible for the quantum phase transition between nonmagnetic Kondo singlet phase and magnetic phase such as observed in many 4f compounds. They may be described by Kondo lattice and simplified Kondo necklace type models. Their quantum phase transitions are investigated by numerical exact diagonalization and analytical bond operator methods respectively.

Keywords: quantized spin models, band and itinerant models, valence fluctuation, Kondo lattice, heavy-fermion phenomena

1. Introduction
Interacting many particle systems of condensed matter tend to exhibit broken symmetry states at low temperatures. The molecular field associated with the order parameter then leads to a strong reduction of the entropy per particle in the ordered phase. Frequently the order is of the diagonal charge- or spin-density wave (CDW, SDW) type which may appear in itinerant (metallic) as well as localized (insulating) compounds. However it is possible that the presence of 'frustration' in the system prevents the appearance of order or shifts it to much lower temperature.

Frustration means that the pairwise interactions of particles or spins cannot all be minimized simultaneously in any microscopic configuration. This can occur for the exchange interaction of spin pairs or the inter-site Coulomb repulsion of itinerant electrons. The frustration effect may arise already in the case of nearest neighbor interactions when the lattice has the property of geometric frustration like, e.g. trigonal, Kagomé, checkerboard or pyrochlore type lattices [1]. In this case the fundamental building blocks like triangles, plaquettes or tetrahedrons share common sites such that there is no unique state which minimizes all bond energies to nearest neighbor sites. Consequently there will be many states which have approximately equally low energies, i.e., frustration leads to a large degeneracy of low lying states. This entails large quantum fluctuations which prevent the appearance of long range order. For example a large number of Cu-oxide and halide compounds with $S=1/2$ Cu$^{2+}$ spins fall into this class of magnetically frustrated systems. Likewise mixed valent vanadium oxides may exhibit geometric frustration for charge ordering phenomena [2].

Frustration phenomena can also arise through the competition of longer range interactions even on non-frustrated lattices such as, e.g., the 2D square lattice. In both cases a large number of states with broken symmetry exist that have equal or closely classical energies, thus preventing a long range ordered state. Then at low temperatures there are basically two alternatives: quantum fluctuations may select one of the degenerate states as the true ordered state ('order by disorder') or they may lead to an ordered quantum phase with a new type of order parameter that is of the 'hidden order' type, i.e. it does not display a macroscopic modulation of charge or spin density.

It is still not clear whether frustrated spin systems may also exhibit a true spin liquid ground state with excitation gap and only short range correlations. One of the best candidates is the spin 1/2 n.n. Heisenberg model on a Kagomé lattice [3]. On the other hand the
n.n. Heisenberg model on the less frustrated trigonal lattice has a magnetic ground state [4] with the classical 120° structure while the ground state of the same model in the nonfrustrated square lattice is of the Néel AF type. In both cases however the staggered moment is reduced from its classical value due to zero point quantum fluctuations.

On the 2D square lattice frustration may be introduced by including n.n. exchange interactions as described by the \( J_1 - J_2 \) model. It has a rich phase diagram due to the competition of \( J_1 \) exchange bonds (along sides) and \( J_2 \) bonds (along diagonals) [5, 6]. Depending on the ratio of \( J_1 / J_2 \) both magnetic ground states and magnetically disordered states and quantum phase transitions between them are possible. However, the latter are not genuine spin liquid states but rather display ‘hidden order’ of stacked dimer [7, 8] or spin-nematic [9] type. These phases are stabilized by quantum fluctuations which prevent the appearance of magnetic order. The importance of quantum fluctuations in such frustrated systems is clearly seen in the nonlinear magnetization curves [10] which even may exhibit plateaux, and in anomalous magnetoelastic properties which are related to the peculiar dispersion of spin excitations caused by frustration.

The concept and meaning of frustration is much harder to identify in itinerant electron systems. Let us consider non-interacting electrons described by a n.n. tight binding Hamiltonian on a pyrochlore lattice, or its 2D projection, the checkerboard lattice. The kinetic energy alone cannot be ‘frustrated’ since the hopping element \( t \) is always the same for each n.n. bond. Frustation emerges when one includes electron correlations, e.g. an on-site Coulomb repulsion \( U \) or an inter-site repulsion \( V \). In the former case and in the limit \( U \gg t \) for a half-filled band local moments appear and the exchange energies \( \left( J \sim t^2 / U \right) \) of corner-sharing exchange bonds will be frustrated due to the lattice geometry. This property emerges gradually as \( U/t \) increases. For moderate correlations \( U \leq t \) it is better to look at the staggered susceptibility. Geometric frustration may lead to a ‘flat’ appearance in momentum space and therefore the interacting susceptibility will be enhanced over a very large region in \( q \)-space. This may be interpreted as the signature of frustration in an itinerant system. One famous example is the metallic spinel \( \text{LiV}_2\text{O}_4 \). The associated softening of spin fluctuation modes in a large part of the Brillouin zone leads to large quasiparticle mass enhancement and therefore to large specific heat \( \gamma \)-coefficient and susceptibility at low temperatures [11]. Thus geometric frustration may lead to a novel type of (3d-) heavy fermion state in this compound which is not due to the usual Anderson- or Kondo lattice scenario.

The latter class of heavy fermion systems is usually formed among intermetallic 4f-/5f- electron compounds. They have frequently cubic or tetragonal structures where geometric frustration does not play a role. Nevertheless one may have a quantum phase transition between magnetically ordered and nonmagnetic heavy fermion ground state. At the core is the competition between the on-site Kondo interaction which prefers the singlet state and an induced inter-site RKKY interaction. In a simplified approach due to Doniach[12] the itinerant Kondo-lattice model may be simulated by a pure spin model where the hopping term is replaced by an intersite spin interaction. In this ‘Kondo-necklace’ type model charge degrees of freedom are eliminated because they are not essential for the competition between nonmagnetic singlet and antiferromagnetic (AF) ordered phase. This competition has been studied both with approximate analytical techniques [13, 14, 15] as well as numerical methods [16].

In this article we first discuss the effects of frustration in the local moment \( J_1-J_2 \) model on the 2D square lattice, using both exact diagonalization with finite temperature Lanczos method (FTLM) for finite clusters as well as analytical spin wave methods. In particular the high field magnetization and magnetocaloric effect in the various phases are investigated (Sec. 2) which are relevant for a class of layered vanadium oxide compounds. A theory for the itinerant frustrated 3d- heavy fermion compound \( \text{LiV}_2\text{O}_4 \) will be discussed in Sec. 3. It is based on ab-initio LDA calculations and the self-consistent renormalization (SCR) approach [17, 18]. It will be used to explain inelastic neutron scattering results which give a direct insight into the origin of frustration in this compound. Furthermore in Sec. 4 the quantum phase transitions in Kondo compounds due to competition of on-site Kondo and inter-site RKKY exchange will be investigated. This central problem of f-electron heavy fermion compounds will be discussed using exact diagonalization methods as well as the analytical bond operator approach. Finally Sec. 5 gives a summary and an outlook.

2. Frustrated \( J_1-J_2 \) magnetism on the square lattice

The idea of a possible RVB state in the cuprates has led to a search for quantum spin liquids in 2D antiferromagnetic \( S=1/2 \) compounds. In reality most of them exhibit an ordered state with either antiferromagnetic or exotic hidden order. In particular the n.n. Heisenberg model on a square lattice has the Néel AF ground state. As mentioned before only Kagomé compounds remain as serious candidates for the spin liquid state. Possibly the best studied 2D QAF is the spin-1/2 \( J_1 - J_2 \) Heisenberg model having a control parameter \( J_1 / J_2 \) which may destabilize the Néel-AF state of the \( J_2 = 0 \) Heisenberg model. It will be shown that this leads to various other magnetically ordered or hidden order states comprising a rich phase diagram in the \( J_1 - J_2 \) plane. They also have an interesting behaviour in an external field depending on the amount of frustration which is controlled by \( J_1 / J_2 \). Recently various...
layered vanadium compounds have been found which correspond well to the $J_1$-$J_2$ model. They are of the type Li$_2$VOX$_2$ (X = Si, Ge) [19, 20, 21] and AA'O (PO$_4$)$_2$ (A, A' = Pb, Zn, Sr, Ba) [22, 23, 24] and consist of V-oxide pyramid layers containing V$^{4+}$ ions with S=1/2. From the analysis of zero field thermodynamic results their wave vectors are $Q = (0,1)$ or (1,0) and (1,1) (in units of $\pi/a$) respectively. The boundary between FM and NAF phase is the line $J_1 = 0$, $J_2 < 0$. Other classical phase boundaries are $J_2 / J_1 = 0.5$ (NAF/CAF) and $J_2 / J_1 = -0.5$ (CAF/FM) which lie within the grey sectors. The range of the latter ($J_2 / J_1$ values indicated outside) shows the region of exotic phases stabilized by quantum effects: stacked-dimer phase (right sector) and spin-nematic phase (left sector). Dashed lines correspond to the experimental $\Theta_{CW} = (J_1 + J_2) / k_B$ and refer to the known $J_1$ - $J_2$ compounds [23, 24]. Two solutions $\phi$ (CAF) and $\phi$ (NAF) are compatible with the thermodynamic properties. The former are chosen according to neutron scattering results for Li- and Pb- compounds. (From Refs. [5,6]).

This model has three possible classical magnetic ground states (see Fig. 1) depending on $\phi$: Ferromagnet (FM), Néel antiferromagnet (NAF) and collinear antiferromagnet (CAF) [5]. The influence of exchange frustration leading to enhanced quantum fluctuations is strongest at the classical phase boundaries where the CAF phase joins the NAF ($J_2 / J_1 = 0.5$, $\phi = 0.15\pi$) or FM ($J_2 / J_1 = -0.5$, $\phi = 0.85\pi$) phases. In fact in these regions they are believed to destroy long-range magnetic order and establish two new ordered states, namely a columnar dimer state with a spin gap at CAF/NAF boundary [7, 8, 25, 26, 27] and a gapless spin nematic state at the CAF/FM boundary [9] as shown by the grey sectors in Fig 1. It can be seen already within spin wave approximation that the magnetic order breaks down in this regime since the sublattice moment reduction due to quantum fluctuations diverges close to the two boundary regions [5].

2.1. The $J_1$-$J_2$ model and its phases

The 2D square lattice $J_1$ - $J_2$ model in an external magnetic field H is given by

$$ H = J_1 \sum_{\langle ij \rangle_1} S_i \cdot S_j + J_2 \sum_{\langle ij \rangle_2} S_i \cdot S_j - J h \sum_i S_i^z , $$ \hspace{1cm} (1)

Here $J_1$ and $J_2$ are two exchange constants between nearest and next neighbors on a square lattice, respectively. The exchange parameters are defined per exchange bond. Furthermore the convention $h = g \mu_B H$ ($g$ = gyromagnetic ratio, $\mu_B$ = Bohr magneton) is used. The phase diagram is preferably characterized by introducing equivalent parameters

$$ J_c = (J_1^2 + J_2^2)^{1/2}, \quad \phi = \tan^{-1}(J_2 / J_1), $$ \hspace{1cm} (2)

or $j = \tan \phi = J_2 / J_1$. The angle $\phi$ determines the degree of magnetic frustration.

Figure 1. Left: Ratio of the Curie-Weiss temperature $\Theta_{CW}$ to the maximum position $T_\chi$ of $\chi(T)$ as a function of $\phi$. Open (solid) circles denote the results for 20-site (16-site) clusters, the dotted line corresponds to eight-site cluster. The thin lines indicate experimental values $\Theta_{CW} = 0.49, 1.39, 1.49$ for Pb$_2$VO(PO$_4$)$_2$ (solid) [22], Li$_2$VOSiO$_4$ (dashed) [20], and Li$_2$VOGeO$_4$ (long-dashed) [20], respectively. Right: Phases of the spin-1/2 2D square lattice $J_1$ - $J_2$ model as function of $\phi$ or $J_2 / J_1$. The CAF and NAF order is indicated by arrows, their wave vectors are $Q = (0,1)$ or (1,0) and (1,1) (in units of $\pi/a$) respectively. The boundary between FM and NAF phase is the line $J_1 = 0$, $J_2 < 0$. Other classical phase boundaries are $J_2 / J_1 = 0.5$ (NAF/CAF) and $J_2 / J_1 = -0.5$ (CAF/FM) which lie within the grey sectors. The range of the latter ($J_2 / J_1$ values indicated outside) shows the region of exotic phases stabilized by quantum effects: stacked-dimer phase (right sector) and spin-nematic phase (left sector). Dashed lines correspond to the experimental $\Theta_{CW} = (J_1 + J_2) / k_B$ and refer to the known $J_1$ - $J_2$ compounds [23, 24]. Two solutions $\phi$ (CAF) and $\phi$ (NAF) are compatible with the thermodynamic properties. The former are chosen according to neutron scattering results for Li- and Pb- compounds. (From Refs. [5,6]).

2.2. Thermodynamics and high field properties of the $J_1$ - $J_2$ model

For a compound described by this model it is most important to determine the energy scale $J_c$ and especially its frustration parameter $\phi$. In a simple procedure $J_c = (J_1^2 + J_2^2)^{1/2}$ is obtained from the high temperature specific heat $C_v (T)$ or the temperature $T_c$ where the susceptibility $\chi(T)$ attains its maximum. Furthermore the high-temperature expansion ($T \ll J_c$) yields the Curie-Weiss constant $\Theta_{CW} = (J_1 + J_2)$. Both $T_c$ and $\Theta_{CW}$ can be
here \( \langle \ldots \rangle \) is the thermal average, \( S^z_{\text{tot}} \) the \( z \) component of the total spin of the system, and \( N, N_z \) are the number of sites and the Avogadro constant respectively, \( \mu_0 \) the magnetic permeability and \( k_B \) the Boltzmann constant. In the zero-field case we have \( \langle S^z_{\text{tot}} \rangle = 0 \). These quantities may be computed for finite clusters using the FTLM method (the expressions are also valid in a finite field). The numerically obtained maximum position \( T_f \) of \( \chi(T) \) may be combined with \( \Theta_{\text{CW}} = (J_1 + J_2) / T_f \) to the quantity \( \Theta_{\text{CW}} / T_f \) for comparison with experiment. This quantity is shown in Fig. 1 (left panel) as function of \( \phi \) together with the experimental results for a few \( J_1, J_2 \) compounds. It is seen that no unique solution exists but two (theoretical) frustration angles (intersection points) \( \phi \) (NAF region) and \( \phi \) (CAF region) are compatible with experimental results (straight line) for each compound.

Thermodynamic methods alone cannot distinguish between the two choices. One possibility is to measure the magnetic structure factor \( S(q) \) in diffuse neutron scattering. From the wave vector of the scattering peak one may distinguish between NAF \( (Q = (\pi, \pi)) \) and CAF \( (Q = (\pi, 0), (0, \pi)) \). This has sofar been achieved only for the Pb- and Li- compounds where indeed the CAF phase is realized [30]. For the other compounds no definite answer is known. Since they all belong to the same families one may conjecture that all compounds lie in the CAF sector as has indeed been assumed in Fig. 1 (right).

2.3. Magnetization and saturation fields

Further insight into the possible ground states of the model may be gained by investigation of the uniform magnetization [10]. It may be obtained both from numerical Lanczos calculations as well as analytical spin wave expansion starting from the three ordered magnetic phases. In the latter approach a Holstein-Primakoff (HP) transformation leads to a harmonic spin wave Hamiltonian

\[
H = NE_0 + NE_{\text{zp}} + \sum_{\lambda k} \varepsilon\lambda k (h) \alpha^\dagger\lambda k \alpha_{\lambda k} ,
\]

here \( \alpha_{\lambda k}^\dagger \) are magnon operators that obey bosonic commutation rules. The \( \varepsilon\lambda k (h) \) denote the spin wave dispersion of branch \( \lambda = \pm \) as defined in the appropriate NAF or CAF magnetic Brillouin zone (BZ). Due to symmetry \( \varepsilon\lambda k (k + Q) = \varepsilon\pm k (k) \) in each magnetic phase. Therefore we may define \( \varepsilon_{\lambda k} = \varepsilon_{\pm k} \) and extend the \( k \) summation over the whole paramagnetic BZ. We have

\[
\varepsilon_k (h) = S (a_k + c_k) 1/2 \left( a_k + c_k \cos \theta_k \right) 1/2 ,
\]

where \( \theta_k / 2 \) is the field-induced canting angle of sublattice moments (counted from the field direction) with \( \theta_k = \pi / 2 \) for \( h = 0 \) and \( \theta_k = 0 \) for \( h \geq h_s \) where

\( h_s (J_1, \phi) \) is the saturation field (see upper inset of Fig. 2). For \( h < h_s \) minimization of the mean field energy \( E_0 (h, \theta_k) \) leads to the ‘classical’ canting angle...

---

**Figure 2.** Magnetization curves \( \mu / \mu_0 = g_m = m / S \) for various frustration angles in the antiferromagnetic or disordered sectors (each curve offset by 0.2). Symbols are obtained from \( T = 0 \) Lanczos results for \( N = 16 \) (squares), 20 (diamonds), 24 (dots, circles) size clusters using the Bonner-Fisher construction [28]. Lines are obtained from first order spin wave calculations. Angles \( \phi / \pi = 0.75, -0.21 \) correspond to the possible CAF or NAF values of the Sr compound.

Magnetization curves strongly differ in the extent of nonlinear deviation from the classical curve which corresponds to \( \phi / \pi = -0.5 \). The cases \( \phi / \pi = 0.41, -0.17 \) are deeply within the CAF or NAF regions and overall agreement of spin wave and Lanczos calculations is good. The values \( \phi / \pi = 0.75, 0.17 \) correspond to regions close to or within the nonmagnetic sectors. Close to the CAF/FM boundary the first order spin wave results overemphasize the nonlinear behaviour and become unstable at very low fields. Close to the CAF/NAF boundary the numerical data exhibit a plateau at \( m / S = \mu / \mu_0 = 0.5 \) (see also Ref. [29]). Lower inset shows the position of plotted \( \phi \) values in the phase diagram. Upper inset shows the saturation field as function of \( \phi \) (\( h_s = g_m H_{\text{sat}} \)). (From Ref. [10])

---

determined from the experiment. On the other hand the temperature dependence of \( C_V (T) \) and \( \chi(T) \) may be obtained directly from the defining expressions (in absolute units)

\[
\chi(T) = \frac{N_A \mu_0 g^2 \mu_B^2}{Nk_B} \frac{1}{T} \left( \langle S^z_{\text{tot}} \rangle^2 - \langle S^z_{\text{tot}} \rangle^2 \right), \tag{3}
\]

\[
C_V (T) = \frac{N_A}{Nk_B} \frac{1}{T^2} \left( \langle H^2 \rangle - \langle H \rangle^2 \right), \tag{4}
\]
The sublattice coupling energies are given by
\[ a_k = 4[J_1 - J_2(1 - \gamma_k)], \quad (NAF) \]
\[ c_k = -b_y = 4J_1\gamma_k, \quad \]
\[ a_k = 2[2J_2 + J_1\gamma_y], \quad (CAF) \]
\[ c_k = -b_y = 2[J_1 + 2J_2\gamma_y]y_x, \quad \]
for the two AF phases. Here the momentum structure factors are defined by
\[ \gamma_k = \frac{1}{2}\cos k_x + \cos k_y, \]
\[ \bar{\gamma}_k = \cos k_x \cos k_y, \]
\[ \gamma_x = \cos k_x, \]
\[ \gamma_y = \cos k_y. \]

In Eq. (5) \( E_{ZP} \) is the energy of zero point fluctuations per site:
\[ E_{ZP} = \frac{1}{2N} \sum_{\delta k}\left[ \varepsilon_\delta k(h) - S\delta k \right]. \]

The zero point energy connected with spin waves will lead to quantum corrections in the magnetization which modify the linear classical behaviour. They are obtained from the derivative \( m_{ZP} = -(\partial E_{ZP}(h) / \partial h) \) which is determined by the dispersion \( \varepsilon_k(h) \).

At the classical phase boundaries CAF/NAF and CAF/FM the dispersion becomes very anomalous [5]. It is constant (zero for \( h \leq h_s \)) along lines in the BZ connecting the two competing ordering vectors \( Q \) at the phase boundary [5].

The expression for the magnetization including quantum corrections up to order \( 1/S \) is given by
\[ m = \frac{h}{h_s}[1 - \frac{1}{N} \sum_k c_k \left( \frac{a_k + c_k \cos \theta_k}{2} \right)^2], \]
where on the r.h.s. the classical value of \( \theta \) given by \( \cos(\theta_k/2) = h / h_s \) has to be used. Because \( h_s \approx S \) the second term in Eq. (9) is formally a \( 1 / S \) correction to the linear classical term \( m_0 = S (h / h_s) \). It may be expected that these corrections depend on the degree of frustration measured by \( \phi \).

In the strongly frustrated regime around the classical phase boundaries the dispersion becomes flat along lines in the BZ, thus dramatically increasing the phase space for quantum fluctuations. Hence in these regions of \( \phi \) (shaded areas in Fig. 1 (right)) the deviations from linear classical magnetization should be marked. This is indeed observed in Fig. 2 where magnetization curves both from spin wave calculations and \( T=0 \) Lanczos results are plotted for various frustration angles. Deep within the magnetic regimes the agreement is very good and nonlinear corrections rather weak. However at the phase boundaries CAF/NAF and CAF/FM strong deviations from classical behaviour occur.

On the right side a plateau appears which is due to the gap formation in the dimerized phase. On the left side the magnetization is very nonlinear and spin wave approximation breaks down well before the phase boundary is reached (as seen from the instability in the magnetization at low fields).

From numerical work it was concluded [9] that a gapless spin-nematic phase, i.e., a non-local quadrupolar order without magnetic moment but with broken spin rotational symmetry is the proper ground state in the left corner of Fig. 2. The spin wave approximation employed here shows that in the two shaded corners the magnetic order breaks down. Higher order \( (1/S)^2 \) corrections do not change that observation [14]. However it does not allow any conclusions about the appearance of the presumably true stacked dimer and spin-nematic quantum phases in these corners.

### 2.4. Magnetocaloric properties

Further insight into the quantum phases of the \( J_1 - J_2 \) model and its high-field behaviour may be gained from its magnetocaloric properties. It is a convenient method to determine precisely the saturation field. In practice the magnetization will be rounded at \( h_s \) whereas the magnetocaloric coefficient (the adiabatic cooling rate) has a sharp anomaly from which \( h_s \) may be obtained. This effect has recently gained special attention in frustrated spin systems such as Kagomé lattices [31, 32, 33]. In these systems dispersionless (local) magnons condense at the saturation field leading to a giant magnetocaloric anomaly. Since the spin wave dispersion in the \( J_1 - J_2 \) model close to the phase boundaries also have flat parts as mentioned above it is interesting to study this effect for the present model. The magnetocaloric coefficient \( \Gamma_{mc} \) is defined as the rate of adiabatic temperature change with external field. Using Maxwell’s relations one obtains

\[ \Gamma_{mc} = \left( \frac{\partial T}{\partial H} \right)_S = \frac{T}{C_V} \left( \frac{\partial S}{\partial H} \right)_T = -\frac{T}{C_V} \left( \frac{\partial m}{\partial T} \right)_H. \]

In a paramagnetic system one has \( \Gamma_{mc}^0 = (H / T) \) due to the scaling behaviour of the free energy. We therefore define \( \Gamma_{mc} = \Gamma_{mc}^0 / \Gamma_{mc}^0 \) as the magnetocaloric enhancement due to spin interaction effects. For the \( J_1 - J_2 \) model \( \Gamma_{mc} \) may be again calculated numerically for finite clusters and compared with the spin wave approximation. The former is obtained from the cumulant expression

\[ \Gamma_{mc} = \left( \frac{\partial T}{\partial H} \right)_S = -g \mu_B^2 \frac{\left\langle HS_{\perp} \right\rangle - \left\langle H \right\rangle \left\langle S_{\perp} \right\rangle}{H^2 - \left\langle H \right\rangle^2}, \]

while the spin wave result may be obtained from Eq. (10) using the temperature gradient

\[ \frac{\partial m}{\partial T} = -\frac{1}{N} \sum_{\delta k} \frac{\varepsilon_{\delta k}(h,k)}{2k_BT^2} \sinh^2 \left[ \frac{\varepsilon_{\delta k}(h,k)}{2k_BT} \right]. \]
and the specific heat
\[
\frac{C_{V}}{T} = \frac{k_B}{N} \sum_{k} \frac{\varepsilon_{k}(h,k)^2}{4(k_B T)^3} \sinh^2 \left( \frac{\varepsilon_{k}(h,k)}{2k_B T} \right).
\]

Evaluating Eq. (12) requires the field gradient of the spin wave dispersion which is given by
\[
\frac{\partial \varepsilon_{k}(h)}{\partial h} = \frac{2S}{h_s} \left( \frac{a_k + c_k}{a_k + c_k \cos \theta_c} \right)^{\frac{1}{2}} \cos \frac{\theta_c}{2}.
\]

The magnetocaloric enhancement ratio in spin wave approximation in comparison with the Lanczos results exhibit qualitatively similar features: A strong upturn and a positive peak just above the saturation field \(h_s\) and for \(T \ll J_s\) a negative coefficient immediately below \(h_s\) [6]. A full quantitative comparison, however, is not reasonable because the harmonic spin wave result diverges logarithmically when \(h \to h_s^+\) and the Lanczos results show strong finite size oscillations for \(h < h_s\). An interesting aspect of the spin wave result is a second sign change and a flat (positive) maximum of \(\Gamma_{mc}\) further below \(h_s\). This is a consequence of the nonmonotonic isentropics below \(h_s\) [6].

It is also instructive to consider the dependence of \(\Gamma_{mc}(h = h_s; \phi)\) on the frustration angle, keeping the field at saturation level where the maximum of \(\Gamma_{mc}\) occurs. Surprisingly the maximum enhancement of the magnetocaloric effect (Fig. 3) (left) occurs in the stable AF regions and not at the classical phase boundaries CAF/NAF and CAF/FM where the quantum phases appear due to strong frustration. In these regions a large degeneracy of low lying states (signified by the flat spin wave dispersion along lines in the BZ) should lead to a strong field dependence of the entropy and, according to Eq. (10) to a large \(\Gamma_{mc}\).

However note that the specific heat \(C_V\) occurs in the denominator of Eq. (10). In Fig. 3 (right) the corresponding \(\phi\) dependence of \(C_V(h = h_s, \phi)\) is presented. It shows a strong enhancement in the quantum phase regions \((\phi \simeq 0.15\pi, \phi \simeq 0.85\pi)\), this overcompensates the increase of the numerator in Eq. (10). Therefore the magnetocaloric enhancement \(\Gamma_{mc}\) is only moderate in these regions while its maxima occurs in the middle of the NAF or CAF phase regions in Fig. 3 (right). The measurement of \(\Gamma_{mc}(h)\) should be an excellent method to determine the saturation field \(h_s\) in the \(J_1 - J_2\) compounds. Their absolute values for the known layered V-oxides are ranged between 10 and 25 T [6].

3. Itinerant frustrated heavy fermion compound LiV\(_2\)O\(_4\)

The metallic spinel compound LiV\(_2\)O\(_4\) is the first 3d-heavy electron system discovered [11]. Below 30 K a large specific heat and Pauli susceptibility enhancement appears, achieving \(\gamma = C / T = 0.4 J / mol K^2\) for the former at the lowest temperatures. The entropy contained in the region up to 60 K is Rh2 suggesting that primarily V spin degrees of freedom have to be involved in the formation of heavy quasiparticles. Many proposals to explain this behaviour have been made, including traditional Kondo-like scenarios. A special feature of the spinels and therefore of LiV\(_2\)O\(_4\) is the fact that V atoms reside on a pyrochlore lattice, their average electron count is \(n_d = 1.5\) per V. In a simple tight binding picture this corresponds to quarter-filling (in the hole picture) of d-bands, i.e. the system is far from the

![Figure 3](https://example.com/figure3.png)

**Figure 3.** In this figure the field is kept at the saturation field for every \(\phi\), i.e. \(C_{V}(T,H) = (\partial T / \partial H)\) at the saturation field as a function of the frustration angle \(\phi\) using a fixed temperature \(T = 0.2 J_s / k_B\). The filled circles denote the normalized values \(\Gamma_{mc}(T / H)\), corresponding to the enhancement relative to a paramagnet. Right: Value of the heat capacity \(C_V(T,H)\) at the saturation field as a function of the frustration angle \(\phi\) for a fixed temperature \(T = 0.2 J_s / k_B\). Both plots were made using a 24-site cluster. (From Ref. 6).
3.1. Electronic structure and spin susceptibility

The pyrochlore lattice has four atoms per unit cell. A next neighbor tight binding model for a single orbital [34] leads to four bands where the upper twofold degenerate band is completely flat. The real bandstructure of LiV$_2$O$_4$ keeps a resemblance to this simple model with a very large DOS peak on top. However the Fermi level is far below the top and this peak does not directly play a role for an enhanced $\gamma$-value. Nevertheless the flat upper band is indirectly important within the spin fluctuation mechanism for the mass enhancement. For this model one needs to calculate the dynamic and momentum dependent spin susceptibility. Starting from the ab-initio LDA bands this is a formidable task [17] due to the large number of d-orbitals and four atoms per unit cell. Assuming only local exchange interactions between electrons the susceptibility of the interacting system is then obtained within RPA type approximation.

The result of this calculation for various subcritical exchange strengths is shown in Fig. 4 for the [111]- and [110]- direction in momentum space. It shows surprisingly that the susceptibility is enhanced by approximately the same factor in a nearly spherical region with a radius $Q_c \approx 0.6\AA^{-1}$ and a finite thickness $\delta Q \approx 0.45\AA^{-1}$ within the momentum space. This is the signature of frustration for itinerant spin fluctuations. Since the static $\chi(Q) \approx \chi(Q_c)$ is almost degenerate in this shell it means that the system, although close a magnetic instability has no obvious way to select an ordering wave vector. As a consequence the dynamical susceptibility will show a slowing down (shifting the spectral function weight to very low energies) in the whole critical shell in the BZ. Therefore there is a large phase space of low energy spin fluctuations which can renormalise the quasiparticle mass. This situation is quite different from non-frustrated lattices where the enhancement of the interacting susceptibility is usually sharply peaked around the incipient magnetic ordering vector, providing only a small phase space and moderate quasiparticle mass enhancement through spin fluctuations.

3.2. Mass enhancement and inelastic neutron scattering

When $Q$ is located within the critical shell the dynamical susceptibility which describes low energy spin fluctuations may be approximately written as (Q = $Q_c$)

$$\text{Im} \chi(Q, \omega) \approx z_0 \chi(Q) \omega / \Gamma(Q),$$

(15)

where $\Gamma(Q)$ and $z_0 < 1$ are their energy width and weight respectively. Since $\chi(Q)$ is much enhanced and $\Gamma(Q)$ small in the critical shell the spectral function is strongly peaked at low energies in this region of momentum space. This is precisely what has been found in inelastic neutron scattering (INS) which probe the spectral function $\text{Im} \chi(Q, \omega)$ [35, 36, 37]. A large scattering...
intensity was observed in exactly the same momentum region where the theoretical calculations predict the critical shell of enhanced slow spin fluctuations. The conduction electrons are dressed with these low energy bosonic excitations leading to a large low temperature specific heat. Using this idea the linear specific heat coefficient due to renormalized quasiparticles may be expressed as [17]:
\[
\gamma_\varphi = \frac{k_B \pi}{N} \sum N_z \langle \hat{H}(q) \rangle,
\]
(16)
Since $\Gamma(q)$ is small in the whole critical shell around $|q| = Q_c$ this may lead to a large linear specific heat. The absolute scale of the spin fluctuation width, $\Gamma$ is not well known from INS and is estimated to fall between the limits 0.5 meV $< \Gamma < 1.5$ meV with a corresponding $300 > \gamma_\varphi > 100$ in units of $mJ/K^2mol$. This result shows that slow spin fluctuations over extended momentum region, caused by the effect of frustration, may explain the size of the large $\gamma$ value in LiV$_2$O$_4$ and its heavy fermion character.

3.3. Mode-mode coupling effects
Up to now the spin fluctuations with various momenta $q$ were treated as independent overdamped harmonic oscillators. This is only justified at very low temperatures. At larger temperatures the spin fluctuation modes of different $q$ couple with each other leading to a transfer of spectral weight from the critical region to low momentum region. Experimentally it was observed that above 60 K the susceptibility enhancement in the critical shell around $q = Q_c$ vanishes and becomes equal to the value at $q = 0$.
This effect of mode coupling may be described within Moriya's self-consistent renormalization (SCR) theory [38] where the static susceptibility is described by
\[
\frac{1}{\chi(q, T)} = \frac{1}{\chi(q, 0)} + \tilde{F}_{Q_c} \int_0^{\infty} \frac{d\omega}{2\pi} e^{i\omega t} - \frac{1}{N} \sum_{q} \text{Im} \chi(q', T).
\]
(17)
Here $\tilde{F}_{Q_c}$ is a mode-mode coupling constant for the critical shell of spin fluctuations. Under certain simplifying assumptions the reduced susceptibility may be written as
\[
\chi(Q_c, T) = \frac{1}{2T_A \gamma_{Q_c}^2(T)},
\]
(18)
where $T_A \approx 220$ K is a scale parameter. The reduced inverse susceptibility $\gamma_{Q_c}^2(T)$ is obtained from numerical solution of the SCR integral equation derived from Eq. (17). Due to the peculiar shell structure of the critical region in the present frustrated system this equation is qualitatively different from the usually treated AF of FM case of unfrustrated magnetism.

The resulting temperature dependence of the critical susceptibility $\chi(Q_c, T)$ together with corresponding experimental results and those of $q = 0$ are shown in Fig. 5. It clearly demonstrates that the critical enhancement of $\chi(Q_c, T)$ is rapidly reduced with temperature and approaches that of the FM point $q = 0$.
Since the ratio of scattering intensities at $q = Q_c$ and $q = 0$ is proportional to the square of the susceptibilities Fig. 5 implies that the critical scattering intensity at $Q_c$ is reduced by almost a factor 16 when temperature increases to 60 K. It remains to be seen whether the SCR theory can also explain the T-dependence of NMR relaxation rate and resistivity in LiV$_2$O$_4$.

4. Quantum phase transitions in the Kondo lattice and Kondo necklace type models
An especially important example of a system with competing interactions is the Kondo lattice (KL) model. It is the canonical model to describe the quantum phase transitions between magnetically ordered and heavy Fermi liquid phase in 4f-based heavy fermion systems such as ternary Ce-122 (e.g. CePd$_2$Si$_2$) or Ce-115 (e.g. CeCoIn$_5$) compounds. The origin of competing interactions is more subtle than in localized frustrated spin systems or the geometrically frustrated one-component 3d electron systems. In the 4f intermetallic compounds there are both localized (4f) and itinerant electrons. They are coupled by a local AF exchange interaction which is the result of a Schrieffer-Wolff process that eliminates the 4f-charge fluctuations in the underlying hybridization model. Together with the remaining hopping term of conduction electrons the Kondo lattice model is given by
\[
H_{KL} = i \sum_{i,j, \sigma} c_{i, \sigma}^\dagger c_{j, \sigma}^\dagger + J \sum_i \tau_i \cdot S_i.
\]
(19)
Here, $\tau_i$ and $S_i$ are itinerant and local (f-) spin, respectively. The KL model takes into account hopping of conduction electrons ($t$) and their AF exchange (Kondo) interaction, ($J > 0$) with local f-spins. This
model has a long history with many approximate analytical treatments for which we refer to the monography by Hewson [39]. The special case of the 1D KL model is reviewed in Ref.[40]. There are also numerical attempts to describe the quantum phases of this model like MC simulations [41, 42] and DMFT calculations [43, 44].

Here we focus on two problems: (i) The competition between on-site Kondo singlet formation and induced intersite RKKY correlations. This fundamental microscopic aspect has been investigated with FTLM method for finite clusters [16]. (ii) The quantum phase transition as function of the control parameter \( J/t \) between AF magnetic and Kondo singlet (KS) phase will be studied with an approximate analytical method based on the bond operator formalism. For this purpose the more simple class of Kondo-necklace (KN) type models, which are pure spin models, will be used instead of the original fermionic KL model [13, 14, 15].

4.1. Correlations in the Kondo lattice model studied with FTLM

The KL model has two competing correlations: The on-site Kondo-singlet correlation \( \langle \tau_i S_j \rangle \) between itinerant and local spin which is a measure for the local singlet amplitude and the inter-site correlations \( \langle S_i S_j \rangle \) between local spins which probe the tendency to magnetic order. The latter are correlations which are of the induced RKKY type for small \( J/t \). They have been calculated for a small cluster size \( N=8 \) as function of temperature and control parameter \( J/t \) using FTLM [16]. Because of the large number of states \( 8 \) stes per site) this method is restricted to clusters of less than ten sites. The calculations have been performed for both periodic and open cluster boundary conditions. Only the latter is shown here because in this case the energy distribution of (discrete) free electron states has a closer resemblance to the DOS of the 2D continuum limit [16].

Figure 6. Ground state correlations \((T=0)\) as function of \( J/t \) using open boundary conditions. Circles represent the on-site Kondo correlations and squares the induced inter-site (n.n.) RKKY correlations. Right inset shows the 8-site KL cluster. (From Ref. [16]).

The evolution of correlations as function of the Kondo interaction strength \( J \) is shown in Fig. 4 for the case of open boundary condition. In the free case \((J=0)\) the on-site singlet and induced inter-site RKKY correlations are zero. When \( J \) is turned on the local singlet correlation starts to increase monotonically and for \( J/t \gg 1 \) approaches the strong coupling limit with fully formed Kondo singlet, i.e. \( \langle \tau_i S_i \rangle = \frac{3}{4} \). The induced inter-site correlations for small \( J \) increase even faster, however they reach a maximum quite soon and then are suppressed again due to the on-site singlet formation. Due to this nonmonotonous behaviour a crossing of on-site and inter-site correlation strengths at finite control parameter occurs. This suggests that in the thermodynamic limit a quantum phase transition from a magnetically to a singlet ground state as function of the control parameter is to be expected. This confirms Doniach's idea of quantum phase transitions in the Kondo lattice model and will be discussed further below.

An alternative way to understand the gradual singlet formation with increasing \( J/t \) is to look at the total on-site magnetic moment. It is given by

\[
\langle \mu_{\text{loc}}^2 \rangle = \langle (\tau_i + S_i)^2 \rangle = \langle \tau_i^2 \rangle + \langle S_i^2 \rangle + 2\langle \tau_i S_i \rangle.
\]

(20)

In this expression \( \langle S_i^2 \rangle = \frac{3}{4} \) is constant but the singlet correlation function \( \langle \tau_i S_i \rangle \) evolves with \( J \) according to Fig. 6. Due to the on-site singlet formation conduction electrons become localized and hence the conduction electron moment also depends on \( J \). For \( J=0 \) when conduction electrons are completely delocalized one has \( \langle \tau_i^2 \rangle = \frac{3}{8} \), while in the strong coupling limit it reaches the localized value \( \langle \tau_i^2 \rangle = \frac{3}{4} \). The resulting total moment \( \langle \mu_{\text{loc}}^2 \rangle \) is shown in Fig. 7. It is a good quantity to define a critical value of \( J/t \) at which the crossover from predominantly magnetic to predominantly nonmagnetic ground state occurs. The other possibility would be to compare directly the inter-site and on-site
correlations, however the former depend strongly on the cluster size. Therefore it is preferable to define a critical \( (J / t)_c \) as the value for which \( \langle \mu_{loc}^2 \rangle = \langle \mu_{loc}^2 \rangle_0 / 2 \). Then for open boundary conditions, \( (J / t)_c \approx 1.4 \) (cf. Fig. 7), in good agreement with the values obtained from the Quantum Monte Carlo [41, 45] simulations.

4.2. The Kondo necklace model within bond operator method

The previous small cluster calculations, though very instructive, are naturally still far removed from the thermodynamic limit. If one is focusing on the aspect of the quantum phase transition one may apply an effective simplification. The KL model still contains the charge fluctuations of conduction electrons expressed by the hopping term. It was shown by Doniach [12] that in 1D it may be replaced by an xy-type inter-site exchange term. Thus the KL model is replaced by a pure spin Hamiltonian, the Kondo-necklace (KN) model. In higher dimension this procedure cannot be justified strictly. However suppose we add a Coulomb repulsion \( U_c \) between conduction electrons to the KL model (Eq. (19))

\[
H = t \sum_{\langle i,j \rangle} (\tau_i^x \tau_j^x + \tau_i^y \tau_j^y + \delta \tau_i^z \tau_j^z) + J \sum_{\langle i,j \rangle} (\tau_i^z S_i^z + \tau_j^z S_j^z + \Delta \tau_i^z S_j^z),
\]

In 2D this Hamiltonian is equivalent to a special case of an (anisotropic) bilayer-Heisenberg model [46] where the intra-layer bonds \( t \) are cut in one layer and \( J \) is the inter-layer coupling. Here both spins are 1/2 and the exchange coupling parameters are antiferromagnetic \( (t, J > 0) \). In the above Hamiltonian, \( \tau_i^\alpha \) represent the \( \alpha \)-component of spin of the 'itinerant' electrons and \( S_i^\alpha \) is the \( \alpha \)-component of localized spins at site \( i \).

This model contains anisotropies in the inter-site interaction (\( t \)) and on-site Kondo terms \( (J) \) of Eq. (21). They are characterized by a pair of parameters \((\delta, \Delta)\) respectively. The local anisotropy \( \Delta \) is always present in real Kondo compounds like Ce-based intermetallics due to the crystalline electric field (CEF) and \( \delta \) is caused by spin-orbit coupling of conduction electrons. The quantum phase transitions of this model have been studied both in zero field [13] as function of control parameters \((U, \delta, \Delta)\) and in finite magnetic field [14] as function of field strength. The special case with \((\delta, \Delta) = (0,1)\) has been investigated before in Ref. [47].

An efficient treatment of the KN model starting from the strong coupling \( (J \gg t) \) limit uses the bond operator technique [47]. It is implemented with the transformation [48, 8]

\[
S_{\mu,\alpha} = \frac{1}{2}(s_{\mu,\alpha}^+ + t_{\mu,\alpha}s_{\mu,\alpha} - i\varepsilon_{\alpha}\mu_{\mu,\alpha}n_{\mu,\gamma}),
\]

\[
\tau_{\mu,\alpha} = \frac{1}{2}(-s_{\mu,\alpha} - t_{\mu,\alpha}s_{\mu,\alpha} - i\varepsilon_{\alpha}\mu_{\mu,\alpha}n_{\mu,\gamma}),
\]

where \((\alpha, \beta, \gamma)\) represent the \((x, y, z)\) components and \( \varepsilon \) is the totally antisymmetric tensor. It expresses the original spin operators in terms of bosonic singlet \( (s) \) and triplet operators \( (t_{\mu,\alpha}) \) of a dimer. The latter have to fulfill the bosonic constraint \( s_n^+ + \sum_{\mu} t_{\mu,\alpha}^+ t_{\mu,\alpha} = 1 \).

Using this transformation in the KN model and neglecting higher than bilinear terms in the triplet operators we may apply a mean field approximation by replacing \( s_n \rightarrow \langle s \rangle = \overline{s} \) in the Hamiltonian and simultaneously in the constraint. The latter is added to the KN Hamiltonian introducing a chemical potential for the triplets as Lagrange multiplier. This procedure is appropriate for the nonmagnetic phase where \( \langle t_{\alpha} \rangle = 0 \). It may naturally be generalized to the AF phase (when \( t > t_c \)) with condensed triplets, i.e., \( \langle t_{\alpha} \rangle \neq 0 \). The resulting Hamiltonian may be diagonalized by using a Bogoliubov transformation in the triplet coordinates. One finally obtains the mean field Hamiltonian

\[
H_{mf} = \tilde{E}_0 + \sum_{\mu} \sum_{\alpha=\sigma,\tau} \omega_{\mu,\alpha}(a_{\mu,\alpha}^+ a_{\mu,\alpha} + \frac{1}{2}),
\]

\[
\tilde{E}_0 = -N\left(\frac{2J_s + J_z}{4}(\overline{s}^2 + \frac{1}{2}) + \mu\left(\frac{5}{2} - \overline{s}^2\right)\right),
\]

\[
E_0 = \tilde{E}_0 + \frac{1}{2} \sum_{\alpha} \omega_{\mu,\alpha}.
\]

Here the dispersion of triplet excitations \( \omega_{\mu,\alpha} (\overline{s}, \mu) \) is obtained from the Bogoliubov transformation of the original bilinear mean field Hamiltonian. In addition to the control parameters \( U, J = J_z \) and \((\delta, \Delta)\) it depends on the mean field singlet amplitude \( \overline{s} \) and the chemical potential \( \mu \). In the paramagnetic state \( U(1) \) symmetry with respect to the \( z \)-axis is always preserved therefore one has a twofold degenerate mode \( \omega_{kx} = \omega_{ky} \) and a single mode \( \omega_{kz} \).

Furthermore \( \tilde{E}_0 \) is the (always negative) mean field ground state energy due to the singlet condensation and \( E_0 \) is the total ground state energy containing the zero point fluctuation energy of triplets. \( E_0 \) also depends on the singlet amplitude \( \overline{s} \) and chemical potential \( \mu \) which have to be determined selfconsistently from the extremal
condition \( \partial E_0 / \partial \sigma = 0 \) and \( \partial E_0 / \partial \mu = 0 \). Once they are
known the triplet dispersion may be obtained. Since the
model contains AF inter-site exchange \((t > 0)\) its
minimum is always at the AF point \( Q = (\pi, \pi) \) in 2D.
For xy-type anisotropy \((0 < \delta < 1)\) the lowest mode is
always \( \omega_{xy}^x \). Its minimum at \( Q \) defines the
spin-excitation gap \( E_x \). In the special case \( \Delta = 1 \) for isotropic
on-site Kondo coupling it is given by \( E_g = E_{g,x} = \omega_{xy}^x \) with
\[
E_g = (\mu + J) \sqrt{1 - D(\frac{\sigma^2}{\mu + J/4})},
\]
(24)
where \( D \) is the dimension of the cubic lattice. The size of the
singlet- triplet gap \( E_g \) in general depends on the
control parameters \( t/J \) and \((\delta, \Delta)\). If it vanishes the
triplets will condense and the mean field amplitude
\( T = (t_{Q_x,y}) \) (assuming the easy-plane case \( 0 < \delta < 1 \)) is
related to the AF order parameter according to
\( \langle S_x \rangle_A = -\langle S_x \rangle_B = \sigma T = m_s \) where \( AB \) denote the AF
sublattices. Hence \( E_g(t/J, \delta, \Delta) = 0 \) defines the
quantum critical point (QCP) between the nonmagnetic
Kondo singlet and AF ordered state of the Kondo
necklace model.

The bond operator mean field theory may be easily
generalized to the AF case by writing the triplet operator
as sum of mean field value and fluctuation part
according to \( t_{Q_x,y} = \sqrt{N} \partial_{Q_x,y} + \eta_{Q_x,y} \). Expressing
the KN Hamiltonian again up to \( 2^{nd} \) order in the triplet
fluctuations \( \eta_{Q_x,y} = t_{Q_x,y} \) and performing the Bogoliubov
transformation one obtains the excitation spectrum
\( \omega_{\alpha,\sigma}(\epsilon, T, \mu) \) in the AF ordered phase which is ungapped
due to the presence of a Goldstone mode. The QCP in
this case is defined by the vanishing of the AF order
parameter, i.e. by \( T = 0 \).

In mean field theory it is found that the QCP occurs
only in 2D and 3D while in 1D the singlet phase with a
spin gap always prevails. However for the Ising case
\( \delta > 1 \) this is an artefact of the mean field approximation
[49]. A typical 2D case with \((\delta, \Delta) = (0, 0)\) (full
anisotropy) of the quantum phase transition and
associated QCP is shown in Fig. 8 (left). As \( t/J \) increases
the singlet-triplet gap energy is reduced and vanishes at
\( (t/J)_c = 0.34 \) which separates the KS and AF phases.
Likewise the AF order parameter or staggered moment
\( m_s = \sigma T \) appears at this point. The singlet amplitude
\( \sigma \) and the chemical potential \( \mu \) vary smoothly across the
QCP. The same is true for the split-off noncritical mode
\( \omega_{\alpha c} \) which is also shown. The critical exponents for
\( E_g \) and \( m_s \) defined close to \( t_c \) are 1 and 1/2 respectively as
is to be expected for the mean field approach. To obtain
the true nontrivial exponents one has to use a more
sophisticated theory briefly mentioned below.

However the mean field theory gives quite
satisfactory results for the position \((t/J)_c \) of the QCP.
In the special cases \((\delta, \Delta) = (0, \Delta)\) or \((\delta, 1)\) it may be
explicitly given as
\[
\frac{1}{(t_c/J)_c} = \frac{2D}{1 + \Delta} \left( \frac{\alpha}{2} \right) \sum_{k,\Delta} \frac{1}{1 + \gamma_\alpha(k,D)}.
\]
(25)
For the other cases it can only be obtained numerically
by the condition \( E_g = 0 \) or \( T = 0 \). The full results for
the QCP \((\delta < 1)\) are shown in Fig. 8 (right). The critical
point \((t/J)_c \) depends more strongly on the local
anisotropy because a decrease of \( \Delta \) destabilises the local
Kondo singlet (the singlet-triplet splitting is reduced)
which leads to a reduction of \((t/J)_c \). On the other hand
for \( \Delta = 1 \) the critical point has a cusp-like \( \delta - \)
The zero-field quantum phase transition as function of $t/J$ can experimentally be mimicked by applying hydrostatic or chemical pressure (through alloying), mostly in 4f-based heavy fermion systems. This will change the control parameter and possibly drive the system across the QCP. A more convenient method is the application of an external field leading to the singlet AF phase. iii) For slightly above critical field not only the magnetic order parameter $m_s$ but also the tilting of the moments with respect to field direction $(g_{x},g_{y})=(2,0)$ is used in both plots. (From Ref. [14]).

Furthermore the field directly induces an amplitude $T_{g}$ for the $z$- triplet mode. Therefore the selfconsistent solution for these amplitudes and the chemical potential is more involved but in principle rather similar to the zero field case.

A typical result of the field driven quantum phase transition is shown in Fig. 9 for isotropic and fully anisotropic case (left) and mixed case (right). Three scenarios for the field induced transitions are possible: i) Starting from a subcritical $t < t_c$ with a KS phase at $h=0$ a field induced transition to an AF phase $(m_s > 0)$ at a critical field $h_c$ takes place. This is the most frequently occurring case for a given parameter set $(\delta,\Delta)$ and $(g_s, g_r)$ (see Fig. 9 (left)). ii) Using an above critical $(t/J > (t/J)_c$ the zero-field AF state is destroyed by the application of a magnetic field leading to the singlet KS phase. iii) For slightly above critical $(t/J) \approx (t/J)_c$ an intermediate ('reentrant') phase sequence is possible. Starting from the KS phase the spin gap is rapidly suppressed and the AF phase is induced by a field. At still larger field the AF order parameter is destroyed again and the KS phase reappears. Examples of the second and third case are given in Fig. 9 (right). The latter two scenarios occur only for rather special combination of control parameters. It is worthwhile to mention that in an external field not only the magnetic order parameter $m_s$ but also the tilting of the moments with respect to field direction

\[ H_Z = +\gamma_{c} \sum_{n}(S_{n}^{z}S_{n+1}^{z} + S_{n}^{z}S_{n+1}^{z}) - i \gamma_{s} \sum_{n}(S_{n}^{x}S_{n+1}^{y} - S_{n}^{y}S_{n+1}^{x}), \]  

where $\gamma_{c} = \frac{1}{2}(g_{s} \pm g_{r})\hbar$, $\hbar = \mu_{B}H$ and $g_{s}$, $g_{r}$ are the gyromagnetic ratios for localized $(S_{n}^{z})$ and itinerant $(\tau_{m}^{z})$ spins respectively which may be very different. It is reasonable to assume $g_{s} > g_{r}$ since the localized (pseudo) spins in 4f-compounds may have very large g-factors. Including this term in the mean field calculation is technically more demanding because it mixes and splits the $x,y$ triplet modes. One therefore has two define new modes:

\[ h_{n} = -\frac{1}{\sqrt{2}}(t_{nx} - it_{ny}) , \quad d_{n} = \frac{1}{\sqrt{2}}(t_{nx} + it_{ny}) , \]  

with mean field amplitudes $\overrightarrow{\tau}$ and $\overrightarrow{d}$ instead of only $\overrightarrow{T}$. Furthermore the field directly induces an amplitude $T_{g}$ for the $z$- triplet mode. Therefore the selfconsistent solution for these amplitudes and the chemical potential is more involved but in principle rather similar to the zero field case.
changes with field strength [14].

These results may have some relevance for real heavy fermion materials. There mostly the second case, namely the AF-KS phase sequence as function of field strength occurs. One prominent example is YbRh$_2$Si$_2$ which exhibits a AF-KS quantum critical point at low fields with associated non-Fermi liquid behaviour [50]. The first case with a KS-AF phase sequence should occur most frequently according to the analysis of the KN model. However in reality it is most difficult to realise, with CeRhIn$_5$ [51] (under constant bias pressure) being a rare example of a field-induced AF phase out of the KS phase.

Finally we mention that within bond operator method the KN model may be treated beyond mean field approximation by using the hard core boson approach [15]. In this method the singlet-triplet constraint is implemented locally by introducing a hard-core repulsion for triplets rather than globally by using a chemical potential as is done in the mean field case. The hard core term is then treated within a ladder diagram approximation. This more advanced treatment gives slightly improved values for the QCP ($\rho / J_1$). However its main advantage is that one may obtain nontrivial critical exponents of the spin excitation gap close to the QCP. The gap scaling exponent $\nu$ shows considerable dependence on the anisotropy $\delta$. It changes from $\nu \approx 0.82$ for the U(1) case with $(\delta, \Delta) = (0,1)$ to $\nu \approx 0.72$ for the SU(2) symmetric case $(\delta, \Delta) = (1,1)$ [15].

5. Summary and outlook

The study of many body systems with frustrated or competing interactions opens a window to interesting quantum phenomena, notably the existence of hidden order phases stabilized by quantum fluctuations and the possibility of quantum phase transitions caused by tuning a control parameter. In addition in itinerant systems frustration emerges due to correlations which may lead to strong renormalization of electronic quasiparticles.

Of particular interest is the spin nematic hidden order phase in the 2D $J_1-J_2$ model. Such a state has theoretically been postulated many times but never been identified. As can be seen from Fig. 2 some of the layered vanadium compounds lie quite close to the spin nematic sector in the phase diagram and one can hope to reach it through further chemical modification or substitution. Even outside this sector it was found that pronounced anomalies in the magnetization appear. This deserves to be further investigated. There is presently no efficient theoretical method to describe this phase and its excitations besides the numerical analysis[9]. This is an outstanding problem.

It has been proposed that the intriguing 3d-heavy fermion compound LiV$_2$O$_3$ is a frustrated metal close to a magnetic instability. This explains naturally the momentum and temperature dependence of neutron scattering results. The associated slowing down of low lying spin fluctuations in conjunction with the very large instability region in q-space due to frustration effects was found to explain the quasiparticle mass enhancement. It would be desirable to include the effect of intersite charge correlations in this compound which may also be important for the nearly critical behaviour.

The Kondo lattice systems show a different type of competing interactions. The interplay of on-site and induced inter-site exchange is responsible for quantum phase transitions between the Kondo singlet and the AF ordered state. It was found that even in 2D the simplification of the KL model to a spin-only KN model is reasonable. The dependence of the quantum critical point given by $\rho / J_1$ on the model parameters can be fully understood by using the mean field bond operator technique. In a special case it reproduces very accurately the QCP of the fermionic model know from QMC simulations. This technique has also been applied to the magnetic field-driven quantum phase transitions and three possible scenarios were found. Remarkably the one most frequently found in the KN model, namely the field induced AF phase is not so common in real Kondo compounds. The study of critical scaling close to the QCP requires an approach beyond the bond operator mean field theory discussed here.

The KL or KN models have sofar been investigated on simple lattices. Recently Kondo materials with underlying geometrically frustrated lattices have been found. In this case both competing and frustrated interactions should play a role. This is an unsolved and challenging theoretical problem.

Acknowledgement

The author would like to thank I. Eremin, P. Fulde, A. Langari, K. Penc, H. Rezania, B. Schmidt, N. Shannon, T. Takimoto, A. Yaresko, V. Yushankhai, I. Zerec and M. Zhitomirsky for collaboration and discussions on the various subjects of this work.

References


1. S=1 systems with local quadrupole order are not of the true spin- nematic type.