Integer and fractional quantum hall effects in lattice magnets

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Part I

Magnetism and the Double-Exchange Model

CHAPTER 2

INTRODUCTION

2.1 Interacting electrons and spins

The Kondo lattice model (KLM) is probably the most celebrated starting point for the investigation of the interplay between localized spins and itinerant electrons [25]. It provides the canonical explanation for the Kondo effect and for the heavy-fermion behaviour observed in many materials [26]. Furthermore, the KLM and its cousin, the double-exchange (DE) model, have proven very powerful in understanding and explaining the properties of manganese-based oxides. The abundance of relevant literature on this subject is nicely summarized in [27,28]. The manganese ion Mn^{3+} provides perhaps the best example of a (large) local spin interacting with an itinerant conduction electron, which is a consquence of the orbital degeneracy present in $3d$ systems and the particular valence of Mn^{3+}.

Motivated by the search for topologically non-trivial states of matter, several groups have studied the itinerant KLM on frustrated lattices, such as the triangular or the pyrochlore one, and have shown that due to the strong geometrical frustration scalar-chiral types of magnetic ordering emerge [29–33]. In addition, the KLM has rather recently come into focus as a good framework to address unusual transport phenomena in spin ice pyrochlores [34–37].

All these distinct examples highlight the broad relevance and applicability of the KLM to a wide range of material classes.

2.2 Kondo Lattice and Double Exchange models

As already briefly introduced in chapter 1, the simplest Hamiltonian that captures the interaction of itinerant electrons and spins is given by

$$\hat{H} = \sum_{ij} t_{ij} \hat{\psi}^\dagger_{i\sigma} \hat{\psi}_{j\sigma} + J_{\text{Kondo}} \sum_i \vec{\mathcal{S}}_i \cdot \vec{s}_i, \tag{2.1}$$

where $\vec{s}_i$ is the spin of the itinerant electron and $\vec{\mathcal{S}}_i$ represents the localized spin. The coupling may be anti-ferromagnetic (AFM) if $J_{\text{Kondo}} > 0$ or ferromagnetic (FM) if $J_{\text{Kondo}} < 0$. Writing the electron spin in terms of the creation and annihilation operators we arrive at the Hamiltonian

$$\hat{H} = \sum_{ij} t_{ij} \hat{\psi}^\dagger_{i\sigma} \hat{\psi}_{j\sigma} + J_{\text{Kondo}} \sum_i \hat{\psi}^\dagger_{i\sigma} \vec{\mathcal{S}}_i \cdot \vec{\sigma}_{\sigma\sigma'} \hat{\psi}_{i\sigma'}, \tag{2.2}$$

which we may call the quantum Kondo Lattice model. In some cases it is important to include an explicit AFM coupling of the localized spins , i.e. $J_{\text{AFM}} \sum_{ij} \vec{\mathcal{S}}_i \cdot \vec{\mathcal{S}}_j$, in order to capture a strong AFM tendency caused by superexchange processes.

Generally, the electron spin will be coupled to a localized spin of arbitrary length S. In case S becomes large, it makes sense to approximate the local spin degree of freedom by a classical spin variable. The assumption of classical spins is justified in Mn based compounds, for instance, where the electron spin is coupled to a local spin of length $S = 3/2$, consisting of three t_{2g} spins perfectly aligned. In the rest of this chapter we will work from this assumption as well, but just for the moment we keep the theory general and write the combined action of electrons and spins as

$$S[\vec{\mathcal{S}}, \hat{\psi}^\dagger, \hat{\psi}] = S_{\text{s}}[\vec{\mathcal{S}}] + S_{\text{e}}[\vec{\mathcal{S}}, \hat{\psi}^\dagger, \hat{\psi}]. \tag{2.3}$$

In this expression, the variables $\vec{\mathcal{S}}$, $\hat{\psi}^\dagger$ and $\hat{\psi}$ should be understood as spin and fermion coherent states. $S_{\text{s}}[\vec{\mathcal{S}}]$ is the Berry phase term of the spin coherent state path integral, encoding its quantum nature. Its specific form is irrelevant for our purposes as we will proceed to neglect quantum effects of the local spins. The electronic action is simply given by $S_{\text{e}} = \int_0^\beta d\tau [\sum \hat{\psi}^\dagger (\partial_\tau - \mu) \hat{\psi} + \hat{H}]$, with β the inverse temperature. With this action the partition function reads

$$Z = \int \mathcal{D}[\vec{\mathcal{S}}] \int \mathcal{D}[\hat{\psi}^\dagger, \hat{\psi}]\, e^{-S_{\text{s}} - S_{\text{e}}} \tag{2.4}$$

Indeed, for large spins S it is justified to neglect the time depedence of the spin field and the Berry phase term S_{s}, and one is left with a bilinear fermionic action coupled

to a classical time-independent field. Such an action is similar in its structure to a Hubbard-Stratonovich decoupled Hubbard model with space-time dependent spin quantization axis [38, 39], and as a result may be used to describe a very broad class of phenomena. In the present case, where we model the interaction of electrons and spins, we can use the bilinearity of the action to calculate the fermionic trace exactly,

$$Z_{\mathrm{e}} = \int \mathcal{D}[\hat{\psi}^{\dagger}, \hat{\psi}] e^{-\sum_{x,x'} \bar{\psi}(x)\hat{G}^{-1}(x,x')\psi(x')} = \mathrm{Det}\,[\hat{G}^{-1}]. \tag{2.5}$$

The determinant still depends on the spin fields and the full partition function requires an integration over the spin variables. For brevity we have collected all indices in the variable x. The full fermionic Green's function can be decomposed as

$$\hat{G}^{-1}(x,x') = \hat{G}_0^{-1}(x,x') + \hat{K}(x,x'), \tag{2.6}$$

where $\hat{G}_0^{-1}(x,x')$ denotes the free electron Green's function (when they are not interacting with the classical spins), and $\hat{K}(x,x')$ denotes the Kondo coupling controlled by J_{Kondo}.

Calculating the full partition function is still a difficult problem, even though we can evaluate the fermionic trace in principle. In order to extract information from the partition function and calcualte observables it is necessary to employ approximation schemes. In the following we discuss two limits that will play a key role in the next two chapters. The first is the limit of weak-coupling, where we suppose that $J_{\mathrm{Kondo}}/t \ll 1$. In this limit we may expand the fermionic determinant in the Kondo coupling and obtain an effective free energy for the spins. In the other limit, $t/J_{\mathrm{Kondo}} \ll 1$, allows for a perturbative expansion in the inverse of the Kondo coupling, yielding an effectively spinless Hamiltonian, which depends on the classical spin variables. The latter can be studied by numerical Monto Carlo simulations. We note here that in the case of classical spins the sign of the Kondo coupling is immaterial.

2.2.1 Perturbation in J_{Kondo}/t

In case of weakly coupled conduction electrons and spins, $J_{\mathrm{Kondo}}/t \ll 1$, we can expand the determinant $\mathrm{Det}\,[\hat{G}^{-1}]$ in powers of the small parameter J_{Kondo}/t. An effective action, or free energy F, for the spins can be defined as $e^{-\beta F} = \mathrm{Det}\,[\hat{G}^{-1}]$, from which it easily follows that

$$F = -\frac{1}{\beta} \ln \mathrm{Det}\,[\hat{G}^{-1}] = -\frac{1}{\beta} \mathrm{Tr}\,[\ln \hat{G}^{-1}]. \tag{2.7}$$

Expanding this in the Kondo coupling strength and subtracting the bare electronic part one obtains the general expression

$$F - F_0 = F^{(2)} + F^{(4)} + \mathcal{O}(J_H^6). \tag{2.8}$$

The second order term represents the conduction electron mediated spin-spin interaction and is generally refered to as the Ruderman-Kittel-Kasuya-Yosida (RKKY) interaction. Its explicit form is given by

$$F^{(2)} = -\frac{1}{\beta}\mathrm{Tr}\left[\hat{G}_0\hat{K}\hat{G}_0\hat{K}\right] = -J_{\text{Kondo}}^2 \sum_{\vec{p}} \chi_0(\vec{p})\vec{\mathcal{S}}(\vec{p})\cdot\vec{\mathcal{S}}(-\vec{p}) \tag{2.9}$$

where the sum is over all momenta and

$$\chi_0(\vec{p}) = \sum_{k,i\omega} \hat{G}_0(i\omega,\vec{k}+\vec{p})\hat{G}_0(i\omega,\vec{k})/(\beta N) \tag{2.10}$$

is the susceptibility, with N the number of lattice sites. Since we are dealing with classical spins at this stage, the saddle-point of the spin effective action is simply given by the maximum (or degenerate maxima) of the susceptibility.

In case the non-interacting electronic Fermi surface exhibits special structure, such as nesting at a particular wave-vector $\vec{Q}$, then this will be reflected in the susceptibility. A very illustrative example is the triangular lattice at filling $n = 3/4$, where the bare Fermi surface is hexagon inscribed in the Brillouin zone hexagon [30]. The Fermi surface is nested by three inequivalent momentum vectors which lead to logarithmically diverging susceptibility as function of temperature. The system gains the most energy by using all three degenerate order parameter components equally, as this fully gaps out the Fermi surface. In fact, the divergent susceptibility suggests that electrons will self-organize spontaneously into a spin-density wave composed of the three ordering vectors as a consequence of interactions. A mean-field decoupling of an interacting Hubbard model, where the mean field takes the place of the local moments, can be employed to test this hypothesis, which has indeed been confirmed in case of the triangular and hexagonal lattices [30, 40].

2.2.2 Perturbation in t/J_{Kondo}

If the coupling between conduction electrons and spins is very strong then it makes sense to focus on this Kondo coupling first and then proceed to ask how the itineracy of the electrons alters the picture. It is straightforward to convince oneself that the Kondo term mandates all electronic spins to be perfectly aligned with the local spins. As the sign of the Kondo coupling does not matter for classical spins, we focus on perfect alignment only without loss of generality.

The assumption of perfect alignment of spins is accounted for in a convenient way by defining the spin quantization axis locally on every site. For each site we then has the spin states $|\uparrow,(\theta_i,\phi_i)\rangle$ and $|\downarrow,(\theta_i,\phi_i)\rangle$, where θ_i and ϕ_i are the polar and azimuthal angles representing the spin $\vec{\mathcal{S}}_i$. Transforming to the local quantization is achieved by the $SU(2)$ representation of a rotation of the z axis to $\vec{n} = (\cos\phi_i \sin\theta_i, \sin\phi_i \sin\theta_i, \cos\theta_i)$, which takes the form

$$U(\theta_i,\phi_i) = e^{-i\phi_i\sigma^z/2} e^{-i\theta_i\sigma^y/2}. \tag{2.11}$$

By construction this rotation operator diagonalizes the spin-conduction electron interactions,

$$U(\theta,\phi)\sigma^z U^\dagger(\theta,\phi) = \vec{\mathcal{S}}(\theta,\phi)\cdot\vec{\sigma}, \tag{2.12}$$

at the cost of making the hopping processes spin-dependent in terms of the local quantization. Explicit expressions of the matrix U and the spin-conduction electron interaction $\vec{\mathcal{S}}(\theta,\phi)\cdot\vec{\sigma}$ in terms of the angles (θ_i,ϕ_i) are

$$\begin{aligned}
\vec{\mathcal{S}}(\theta,\phi)\cdot\vec{\sigma} &= \begin{bmatrix} \cos\theta & e^{-i\varphi}\sin\theta \\ e^{i\varphi}\sin\theta & -\cos\theta \end{bmatrix}, \\
U(\theta,\phi) &= \begin{bmatrix} \cos\frac{\theta}{2} & e^{-i\varphi}\sin\frac{\theta}{2} \\ e^{i\varphi}\sin\frac{\theta}{2} & -\cos\frac{\theta}{2} \end{bmatrix}.
\end{aligned} \tag{2.13}$$

With these explicit expression we can evaluate the hopping term in terms of the angles $\{\theta_i,\phi_i\}$. The spin-dependent hopping matrix $t_{ij}^{\sigma\sigma'}$, where σ and σ' label spin-up and spin-down in the local basis, becomes

$$t_{ij}^{\sigma\sigma'} = t_{ij} u_{ij}^{\sigma\sigma'} = t_{ij}\left(U^\dagger(\theta_i,\phi_i)U(\theta_j,\phi_j)\right), \tag{2.14}$$

where the angle-dependence is contained in the $u_{ij}^{\sigma\sigma'}$ functions, which can be read off from the matrix product as

$$\begin{aligned}
u_{ij}^{\sigma\sigma} &= \cos\frac{\theta_i}{2}\cos\frac{\theta_j}{2} + \sin\frac{\theta_i}{2}\sin\frac{\theta_i}{2} e^{i\sigma(\phi_j-\phi_i)} \\
u_{ij}^{\sigma\overline{\sigma}} &= \sigma\left(\cos\frac{\theta_i}{2}\sin\frac{\theta_j}{2} e^{-i\sigma\phi_j} - \sin\frac{\theta_i}{2}\cos\frac{\theta_i}{2} e^{-i\sigma\phi_i}\right).
\end{aligned} \tag{2.15}$$

So far we have not made any approximations but just rewritten the problem in terms of basis states obtained from diagonalizing the spin-conduction electron interaction. Under the assumption that J_{Kondo}/t is very large, we can integrate out the spin-down states, as excitations into the spin-down sector of Hilbert space will be

heavily penalized energetically. Integrating out the spin-down or anti-aligned states yields an effectively spinless Hamtiltonian which reads

$$\hat{H} = \sum_{ij} t_{ij}(\theta_{ij}, \phi_{ij})\hat{\psi}_i^\dagger \hat{\psi}_j + J_{\text{AFM}} \sum_{i,j} \vec{\mathcal{S}}_i \cdot \vec{\mathcal{S}}_j, \tag{2.16}$$

where

$$t_{ij}(\theta_{ij}, \phi_{ij}) \equiv t_{ij} u_{ij}^{\uparrow\uparrow} = t_{ij}(\cos\frac{\theta_i}{2}\cos\frac{\theta_j}{2} + \sin\frac{\theta_i}{2}\sin\frac{\theta_i}{2} e^{i(\phi_j - \phi_i)}). \tag{2.17}$$

An AFM interaction between the localized spins is perturbatively generated at order $\sim t^2/J_{\text{Kondo}}$. This Hamiltonian, given in equation 2.16 is generally refered to as the Double-Exchange (DE) model. It describes electrons strongly interacting with localized spins in such a way that their spin is always tied to the local spin. The kinetic part favors FM alignment of the local spins, as the electrons gain kinetic energy, in such spin configuration. The AFM interaction, which generically models a perturbatively generated interactions between spins, or an intrinsic AFM interaction driven by superexchange, obviously favors anti-ferromagnetism. It is the competition between these two tendencies that is at the heart of the rich and sometimes unexpected physics observed and predicted for systems with spin-electron interactions.

The DE Hamiltonian still depends parametrically on the spins and in order to determine the spin-electron ground state or calcualte correlation functions, one must still integrate over all spin configurations in the partition function. For classical spins the path integral measure is simply an integration over the spin variables $\{\theta_i, \phi_i\}$, i.e.

$$\int \mathcal{D}[\vec{\mathcal{S}}] = \prod_i^N \left(\int_0^\pi d\theta_i \sin\theta_i \int_0^{2\pi} d\phi_i \right) \tag{2.18}$$

Calculating the partition function or correlation functions exactly or even analytically is impossible and one must resort to numerical routines to extract information from the system. The method of choice is classical Monte Carlo where the spin configuration space is sampled according to standard Monte Carlo techniques [27, 28]. In these Monte Carlo simulations, the fermionic problem is diagolized exactly on a finite cluster, which amounts to calculating the fermionic trace in the path integral exactly. The fermionic trace then enters as a weight factor for the sampling of classical spin configurations.