

## **Models in Magnetism: Introduction**

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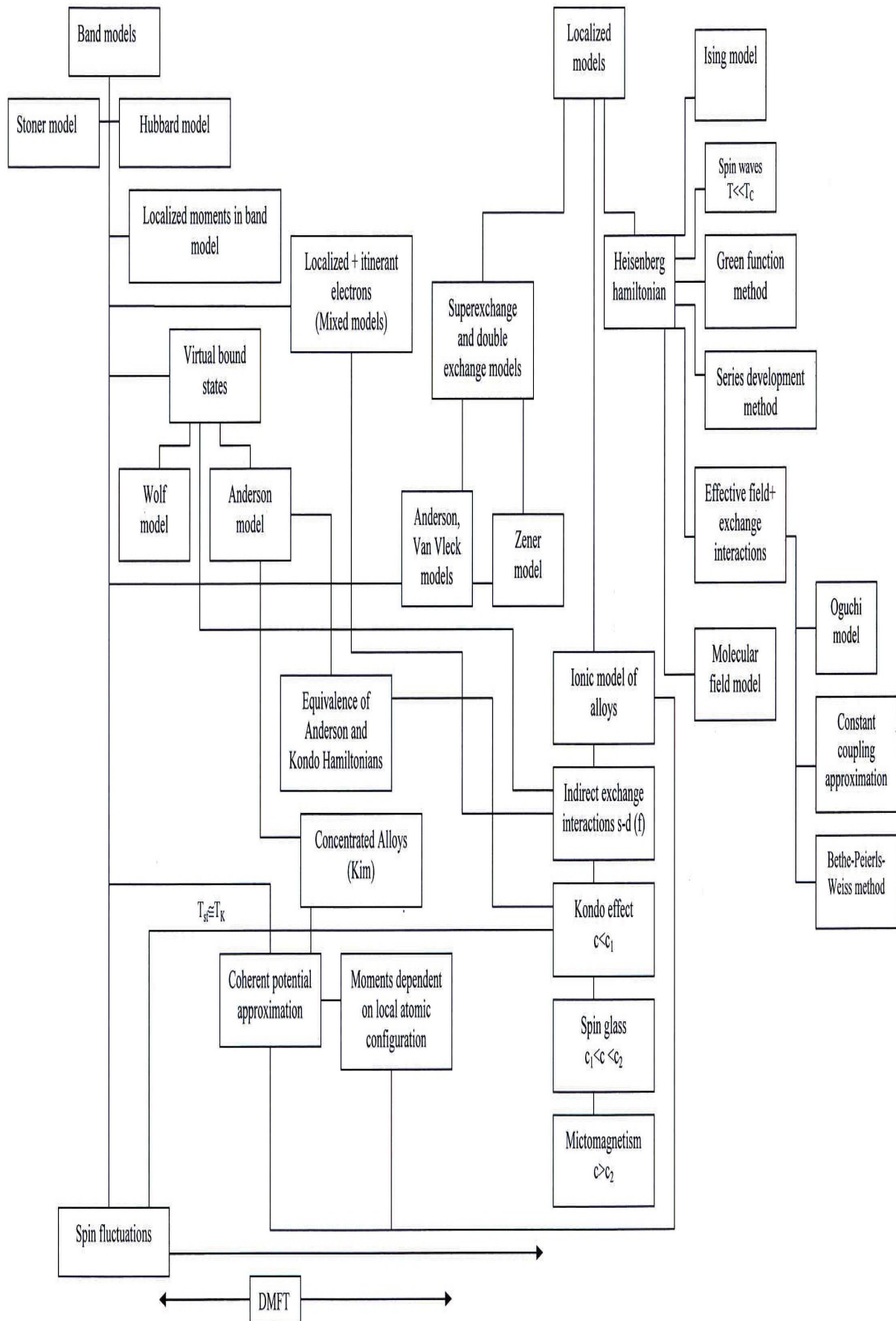
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The present Summer School is focused on the basic problems in magnetism, with the topological developments in the fields. The topics have in view basic concepts, exchange interactions and magnetic ordering, strongly correlated systems, magnetism in reduced dimensions, as well as the effects of coupling with lattice.

In introduction, it is my intention, to present shortly some models used in describing the magnetic behaviour of the matter. This is only a short review on the basic features and of connection between the models, many of these being more depth analysed in the following lectures. A schematic representation of models is given in Fig.1. Two types of basic models, those considering that the magnetic moments are localized at lattice sites and band models, respectively, were elaborated. These are situated in the right part of figure (localized) and left part (band). The models having features from both above descriptions are plotted in the intermediate regions. Herring [1] in the paper “The d electrons states in transition metals”, compared the models used in magnetism, particularly in metallic systems, with cocktails having different ingredients as bands, correlations, coupled atoms and valence bonds. Mixed in different proportions lead to itinerant, minimum polarity, s-d(f) and valence bonds models.

In describing the magnetic properties, there are two independent concepts, namely, the dimensionality of the system,  $d$ , and the number of magnetization components,  $n$ . When the spins are coupled following all the space directions we have  $d=3$ . When the spins are coupled in a plane,  $n=2$  and when the interactions take place along one direction we have  $d=1$  (magnetic chain). A polymer chain has  $d=0$ . Higher values than  $n=3$  are considered in phase transitions description. In the Heisenberg model we have three independent components of magnetization ( $n=3$ ), in X-Y model two ( $n=2$ ) and in Ising model, the magnetization is oriented along one direction ( $n=1$ ). A value  $n=-2$  is characteristic for Gaussian model and  $n \rightarrow \infty$  for a spherical model.

The localized models essentially admit that the magnetic moments are situated on lattice sites. The exchange interactions in metallic systems can be described by direct interactions [2] or by indirect exchange by means of conduction electrons [3]. In magnetic insulators, superexchange [4,5] or double exchange [6] mechanisms were considered.



The short range exchange interactions, commonly, can be described starting from Heisenberg Hamiltonian  $H = \sum_{i,j} J_{ij} \mathbf{S}_i \mathbf{S}_j$ , where  $J_{ij}$  is the exchange integral describing the interactions between the spins  $\mathbf{S}_i$  and  $\mathbf{S}_j$  (only spin moment was considered, as in 3d metals). It is a difficult matter to compute exactly the magnetic properties starting from above Hamiltonian since there we have a many body problem. The Ising model ( $n=1$ ) can be solved exactly in case of unidimensional and some bidimensional lattices. The linear Ising lattice is not ferromagnetic, at finite temperatures. The temperature dependence of the magnetic susceptibility is given by  $\chi \propto T^{-1} \exp(2J/k_B T)$ . In case of quadratic bidimensional lattice, the temperature dependence of magnetization is described by  $M = [1 - (\text{sh} 2k_1 \text{sh} 2k_2)^2]^{1/8}$ , where  $k_1 = J_1/k_B T$  and  $k_2 = J_2/k_B T$ , the  $J_1$  and  $J_2$  being the exchange integrals in the two directions of quadratic lattice [8]. Exact solutions were also obtained for other bidimensional lattices [9]. Rigorous solution has been obtained in spherical Ising model [10]. The predicted magnetic behaviour of tridimensional Ising lattice was analysed by series development methods around the Curie point or at low temperatures.

A class of approximations, starting from Heisenberg Hamiltonian, use the effective field-based analysis. In this case, the exchange interactions between a finite number of spins are exactly solved, while the interactions with the atoms of remaining crystal are replaced by an effective field. When only a single atom is considered, the molecular field approximation model is present [11]. According to Weiss [11], the effective field acting on the atom, in each domain, is proportional to the magnetization,  $M$ ,  $H_{\text{eff}} = N_{ii} M$ , where  $N_{ii}$  is the molecular field coefficient. The  $N_{ii}$  thus introduced, acts at the level of each particle, and ensures the self-consistency. The molecular field coefficient is proportional to the exchange integral  $J_{ij}$  (expected to be the same for a crystal)  $N_{ii} = 2zJ_{ij} (Ng^2 \mu_B^2 \mu_0)^{-1}$ , where  $N$  and  $z$  are the total number and number of neighbouring atoms, respectively. The model predicts, at low temperatures, a dependence of the form  $M(T)/M(0) = 1 - S^{-1} \exp\left(\frac{-3 T_C}{S+1 T}\right) + \dots$  and at temperatures close to Curie point,  $M(T)/M(0) \propto (T_C - T)^\beta$  with  $\beta = 1/2$ . Experimentally was shown, at low temperatures, a  $T^{3/2}$  dependence of magnetization and close to  $T_C$  a value  $\beta = 1/3$ . The model, at  $T > T_C$ , but close to  $T_C$ , gives  $\chi^{-1} = C^{-1} (T - T_C)^\gamma$  with  $\gamma = 1$ , while experimentally a value  $\gamma = 4/3$  was shown.

Fig.1

The above predictions were improved when the exchange interactions between a finite number of atoms were considered, in addition to an effective field, as shown by Néel, Oguchi, Bethe-Peierls-Weiss methods or the constant coupling approximation.

The magnetic behaviour, at low temperatures, in case of localized moments was also analysed in spin wave model. The rigorous solutions of the Heisenberg model, can be obtained if all spins, with exception one, are parallelly aligned. A  $T^{3/2}$  dependence of magnetization is predicted [12], in agreement with many experimental data.

Other approximate solutions of the Heisenberg Hamiltonian were obtained by series development method, around the Curie points or by using the Green function method.

In case of rare-earth metals, the spatial extension of 4f shell is small, unlike the 3d metals. Their properties were described in a s-d(f) model, the interactions between localized moments being realized through the conduction electrons [3]. In the second order approximation of the Hamiltonian, the spin polarization has an oscillatory dependence. The Hamiltonian can be written, in analogy with Heisenberg one, as  $H^{(2)} = \sum J(R_{nm}) S_n S_m$  where  $J(R_{nm}) \propto (\cos k_F R_{nm} - \sin k_F R_{nm}) R_{nm}^{-4}$ . By  $x$  is denoted  $k_F R_{nm}$  where  $R_{nm}$  is the distance between the  $n$  and  $m$  atoms and  $k_F$  is the Fermi wave vector. When both spin and orbital contributions are present  $S$  can be replaced by  $J$ . The model can be used also to analyse the exchange interactions in dilute magnetic alloys.

The band models were also used to describe the magnetic properties of some systems, particularly 3d alloys [13]. These models were elaborated to explain the noninteger number of Bohr magnetons, the presence of 3d bands, having widths of the order of 1 eV as well as the data obtained from transport properties. The presence of the magnetic moment was shown when the Stoner criterion,  $J\eta(E_F) \geq 1$ , is obeyed. By  $J$  is denoted the phenomenological interaction constant between two electrons having parallel spins, defined when the exchange energy of two electrons having antiparallel spins is zero and  $\eta(E_F)$  is the state density at the Fermi level. A  $T^2$  variation of magnetization was predicted, as for example, experimentally observed, in  $ZrZn_2$ .

The Hubbard model [14] is used to describe the magnetic behaviour of transition metals, of their oxides, metal-nonmetal transition as well as magnetic transitions. In this model, the Hamiltonian takes into account the energy of electrons in band and their interaction energy.

There are models which consider both band and localized features as those developed by Friedel [15], Stearns [16] or the Zener modified model [17].

The magnetic properties of dilute 3d magnetic alloys were described in the virtual bound state model of Friedel [18], or by Wolf [19] or Anderson [20] models. These models analyse mainly the formation of magnetic moments on impurity atoms in metallic matrix. Kondo [21] discussed the minimum observed in the temperature dependence of electrical resistivities in dilute magnetic alloys. In the second order of perturbation theory was shown the presence of a logarithmic divergence in scattering of conduction electrons on the local moments. There were also developed models that analysed this divergence at Kondo temperature,  $T_K$ .

An intermediate model, between Heisenberg description of a lattice formed by a single type of atoms and Stoner model, admitting the coexistence of different types of ionic configurations, was elaborated and named “approximation based on ionic configurations” [22].

The analysis of electron correlations effects in d-bands, stimulated the development of spin fluctuations model [23]. According to this model, thermal excitations of electron-hole pair in magnetic materials, have a collective character and are described in terms of spin density fluctuations. In the local moment limit, the spin fluctuations behave like a set of mutually interacting moments with a local character in real space. There are only transverse components of LSF. In weakly ferromagnetic limit or in case of exchange enhanced paramagnets, longitudinal components of LSF or temperature variation of LSF amplitudes play an important role. A local character in reciprocal space has been shown. The intermediate behaviour corresponds to situation when both transverse and longitudinal spin fluctuations are present. The matter of quenching of spin fluctuations by external [24] or internal [25] fields was analysed.

The DMFT combined with standard LDA band calculations [26] showed that in weakly correlated system, the local spin susceptibility is nearly temperature independent, while in a strongly correlated system, Curie-Weiss behaviour can be shown. For an itinerant electron system, the time dependence of the correlation function results in temperature dependence of  $\langle S_{i\alpha}^2 \rangle$ . Fluctuating moments and atomic-like configurations are large at short times. The moment is reduced at longer time scales, corresponding to a more band-like and less correlated electronic structure near the Fermi level.

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