Microscopic mechanisms favoring itinerant ferromagnetism

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Introduction

Ferromagnetism can be stabilized by quite different microscopic mechanisms. Clearly an asymmetric density of states with large spectral weight near one of the band edges is favorable for ferromagnetic order. Nearest-neighbor interactions can also lead to ferromagnetism in a natural way. In an orbitally degenerate two-band model the Hund's rule coupling provides for a third route to ferromagnetism. These three microscopic mechanisms are treated separately on this poster in order to demonstrate differences and common features.

Models

Our starting point for the microscopic description of ferromagnetism is the multi-band Hubbard model which includes kinetic energy and on-site Coulomb interaction.

$$\hat H^{M-\text{Band}}_{\text{Hubbard}} = \sum_{\nu=1}^{M}\sum_{ij\sigma} t_{ij}\,\hat c^{\dagger}_{i\nu\sigma}\hat c_{j\nu\sigma} + U\sum_{\nu=1}^{M}\sum_{i}\hat n_{i\nu\uparrow}\hat n_{i\nu\downarrow}.$$

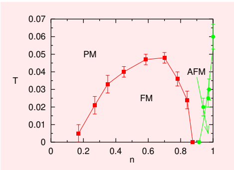
Additional terms are Hund's rule coupling and nearest-neighbor interactions.

Methods

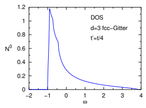
Ferromagnetism is in general an intermediate or strong coupling phenomenon. Only in special cases strong coupling approaches are useful, e.g., for the ferromagnetic insulators triggered by nearest-neighbor interactions at half-filling and by Hund's rule coupling in the orbitally degenerate two-band model at quarter-filling. A more complete picture is here obtained within Dynamical Mean-Field Theory using quantum Monte Carlo simulations. The influence of density-dependent hopping is estimated within Gutzwiller approximation.

Asymmetric density of states

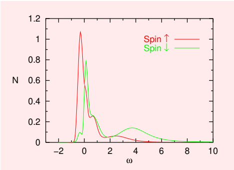
$$\hat H = \hat H^{1-\text{band}}_{\text{Hubbard}} \quad \text{with fcc-DOS}$$



Magnetic T–n phase diagram for asymmetric fcc-DOS $t'=t/4$, $U=6$ (DMFT for $d=3$).



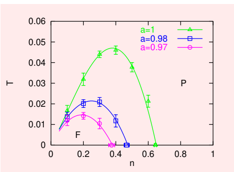
$d=3$ fcc-DOS with $t'=t/4$



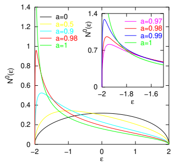
Interacting DOS for $U=4$, $n=0.58$, $T=0.04$.

In the one-band Hubbard model the on-site interaction term U drives the formation of local fluctuating moments. It depends on the form of the kinetic energy whether these moments order magnetically or not.

Apparently a peak near the lower band edge is favorable for ferromagnetism at less than half filling. A singularity (like in the model DOS with $a=1$) is not necessary.



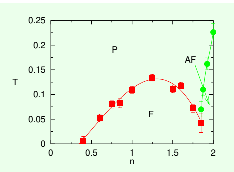
Magnetic T–n phase diagram for asymmetric model DOS and $U=4$.



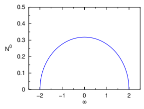
model DOS $N^0(\varepsilon) = c\,\frac{\sqrt{D^2-\varepsilon^2}}{D+a\varepsilon}$ with $c=\frac{1+\sqrt{1-a^2}}{\pi D}$ and bandwidth $2D=4$.

Hund's rule coupling

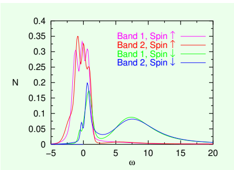
$$\hat H = \hat H^{2-\text{band}}_{\text{Hubbard}} + \sum_{i\sigma\sigma'}(V_0-\delta_{\sigma\sigma'}F_0)\,\hat n_{i,\,\nu=1,\,\sigma}\hat n_{i,\,\nu=2,\,\sigma'}$$



Magnetic T–n phase diagramm for $F_0=4$, $U=9$, and $V_0=5$.



Two degenerate bands with Bethe-DOS $t^*=t\sqrt{Z}\equiv 1$

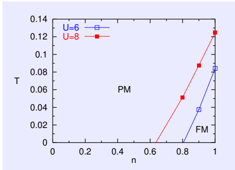


Interacting DOS for $U=9$, $V_0=5$, $F_0=4$, $n=1.25$, and $T=0.09$.

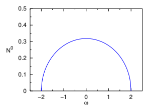
In a multi-band model (e.g., with two degenerate bands) the Hund's rule coupling F_0 can cause ferromagnetism. In addition or alternatively to magnetic order, alternating orbital order can be triggered by V_0.

Nearest-neighbor interactions

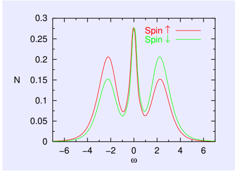
$$\hat H = \hat H^{1-\text{Band}}_{\text{Hubbard}} - 2F\sum_{\langle ij\rangle}\hat{\mathbf S}_i\cdot\hat{\mathbf S}_j + X\sum_{\langle ij\rangle\,\sigma}(\hat c^{\dagger}_{i\sigma}\hat c_{j\sigma}+\text{h.c.})(\hat n_{i,-\sigma}+\hat n_{j,-\sigma})$$



Magnetic T–n phase diagram for $F^*=ZF=0.5$ and $X^*=\sqrt{Z}X=0$.



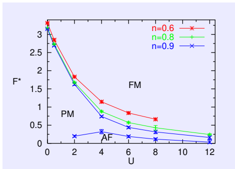
Bethe-DOS with $t^*=t\sqrt{Z}\equiv 1$



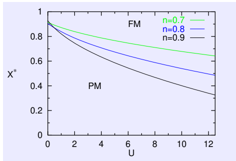
Interacting DOS for $n=1$, $U=6$, $F^*=0.5$, $X=0$, and $T=0.07$.

Expressing the $1/r$ Coulomb interaction in Wannier representation one not only obtains density dependent terms (like the on-site term U), but also the direct exchange term $F\ll U$ between nearest neighbors which can lead to ferromagnetism in a natural way. Another nearest-neighbor term, X, leads to a spin dependent renormalization of the DOS.

Near half-filling strong coupling perturbation theory yields a t–J modell with the effective coupling $J_{\text{eff}}=4(X-t)^2/U-2F$.



Magnetic phase diagram for $T=0$ and $X=0$ (QMC simulation with extrapolation $T\to 0$). For $n\lesssim 0.8$ ferromagnetism is completely suppressed.



Magnetic phase diagram for $T=0$ and $F=0$ in Gutzwiller approximation (AF and SC phases not considered). At very large $U\gtrsim 25$ the Gutzwiller wave function becomes unreliable since it overestimates the energy of the paramagnet.

Conclusion

There are surprising similarities in the phase diagrams and in the (interacting) spectral functions between the models including an asymmetric density of states and Hund's rule coupling, respectively. In both cases the tendency towards ferromagnetism is strongest away from half-filling whereas antiferromagnetism is present at half-filling. This fits in with the experimental situation that Cr and Mn have half-filled bands whereas Fe, Co, and Ni have not.

In contrast both the F term and the X term stabilize ferromagnetism at half filling while suppressing antiferromagnetism.

Hund's rule coupling and/or an asymmetric density of states are the microscopic mechanisms for **itinerant** ferromagnetism.
Nearest-neighbor exchange can change details of the phase diagram, but not be the leading mechanism.

References

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[2] K. Held and D. Vollhardt, cond-mat/9803182 (to appear in Eur. Phys. J. B)

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[4] D. Vollhardt, N. Blümer, K. Held, M. Kollar, J. Schlipf, and M. Ulmke, Z. Phys. B 103, 283 (1997).