Collective Electronic Excitations in Ferromagnetic Metals

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(1) Introduction

- Metal: interacting particle system consisting of lattice ions and valence electrons.

model	assumptions	results
Sommerfeld model	free electrons plane waves	Landau diamagnetism thermodynamics of the free electron gas
Jellium model	interacting electrons plane waves	binding energy of the metallic solid
Hubbard model	interacting electrons Bloch functions	ferromagnetism

- Ferromagnetism is a consequence of strong electron correlations.
- Possible methods: density functional theory DFT or model calculations.

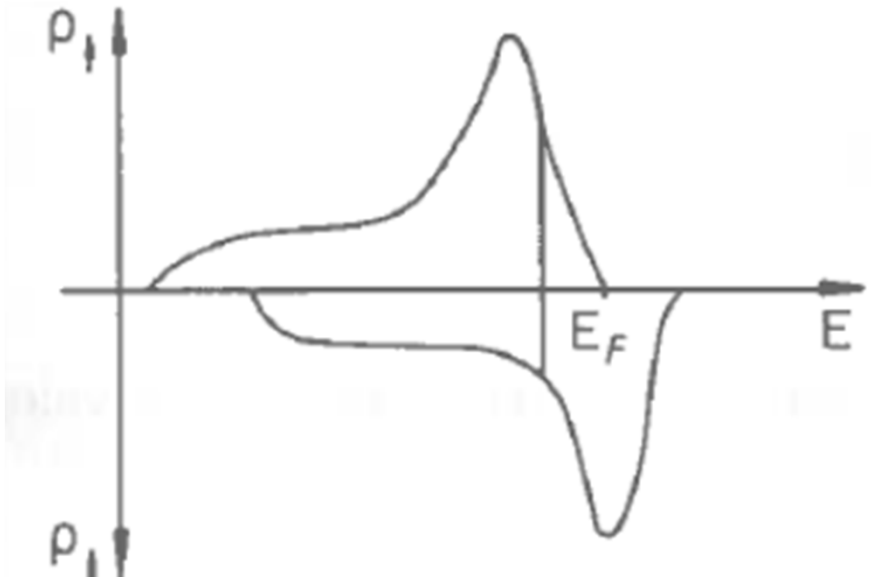
(2) The Model

- Tight binding approximation → Hubbard Hamiltonian.
- $H =$

$$\sum_{ij\sigma}\left(T_{ij} - \mu\,\delta_{ij}\right) a_{i\sigma}{}^{+} a_{j\sigma} + \frac{1}{2}\,U\,\sum_{i\sigma} n_{i\sigma}\, n_{i\,-\sigma}$$

- The Hubbard model explains ferromagnetism on the basis of a spin dependent band shift between the ↑ and ↓ density of states below a critical temperature T_C .

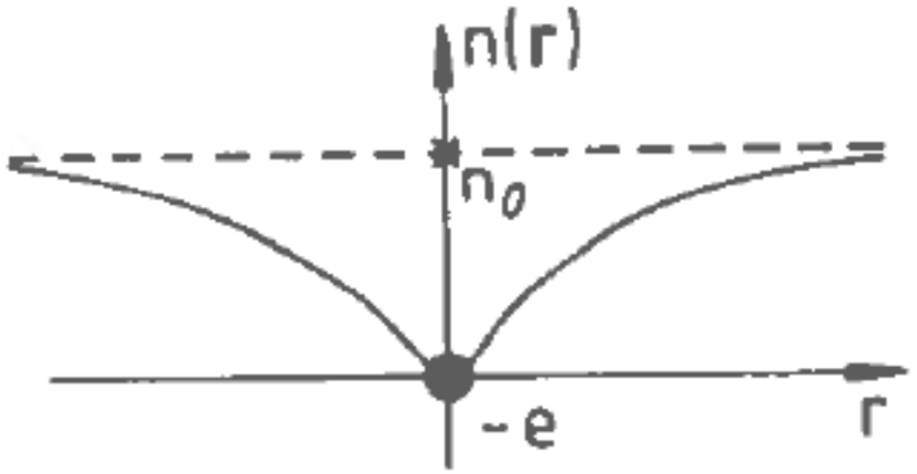
band magnetism: the exchange interaction is responsible for a spin dependent band shift.



- The Hubbard model is a non-trivial many body problem and is in general not exactly solvable. Interesting solutions obtained so far include
- - The Mermin Wagner theorem rules out ferromagnetic order at finite temperatures for $d \leq 2$.
- -For small band occupations n only a paramagnetic solution $n_\uparrow = n_\downarrow = \frac{1}{2} n$ is obtained.
- -In the strong coupling limit $U \gg W$ a saturated ferromagnetic solution is expected for large band occupations n.
- -In the zero band width limit no ferromagnetic solutions are observed.

(3) Charge Density Waves

- Due to charge screening the electron density in a simple metal becomes space vector dependent.

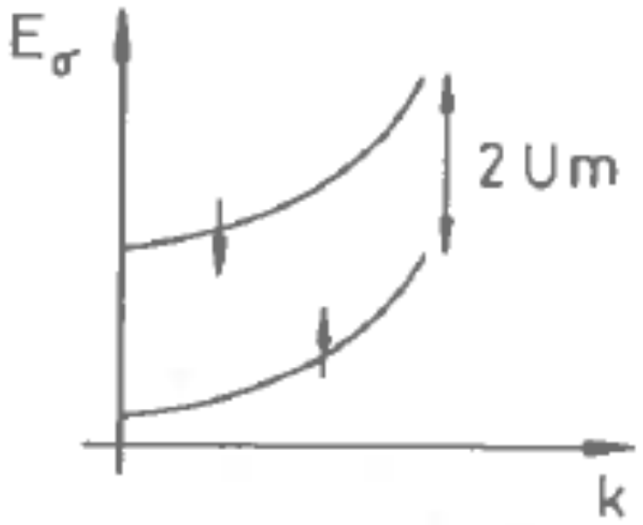


- According to the Thomas-Fermi approximation the eigenenergies can be written in the form
- $E\ (k) = \ \varepsilon\ (k) - e\ \varphi\ (r)$ (1)
- They are obtained from the roots of the dielectric function
- $\varepsilon(\ q, E) = 1\ -\ v_0\ (q) \sum_{k\sigma} \frac{\langle n_{k\sigma}\rangle^{(0)} - \langle n_{k+q,\sigma}\rangle^{(0)}}{E-(\ \varepsilon(k+q)-\ \varepsilon(k))}$ (2)
- The Coulomb potential of the test charge is screened so that the electrons are only subjected to it if their distance r is smaller than the screening range λ_{TF} which is determined from the Poisson equation for the Coulomb potential yielding
- $\lambda_{TF} = \ q^{-1} = \ \sqrt{\frac{2\ \varepsilon_0\ \ \varepsilon_F}{3\ n_0\ e^2}}$
- Furthermore, inserting $\varepsilon\ (\ k) = \ \frac{\hbar^2\ k^2}{2\ m^*}$ into Eq (2) above yields the plasmon frequency
- $\omega_p\ (\ q = 0) = \ \sqrt{\frac{n_0\ \ e^2}{\varepsilon_0\ \ m^*}}$
- and the plasmon energies
- $E_p\ (q = 0) = \ \hbar\ \omega_p\ (q = 0) = \ \hbar\ \sqrt{\frac{n_0\ e^2}{\varepsilon_0\ m^*}}$ (3)
- $4\ eV\ \leq\ E_p\ (q) \leq 25\ eV$
- Plasmons are collective excitations of the free electron gas.

(4) Spin Density Waves

- Diagonal susceptibility within the Hubbard model
- $X_q{}^{zz}(E) = -\frac{\mu_0 \mu_B{}^2}{2V} \quad \frac{\rho_0(\varepsilon_F)}{1 - U\,\rho_0(\varepsilon_F)}$ (4)
- The poles of Eq (4) represent the famous Stoner criterion
- $U \quad \rho_0(\varepsilon_F) \geq 1$
- Transverse susceptibility within the Stoner model
- $X_q{}^{+-}(E) = \frac{\gamma}{N} \quad \sum_k \frac{\langle n_{k+q,\downarrow}\rangle - \langle n_{k\uparrow}\rangle}{E - \Delta E_{\uparrow\downarrow}(k,q)}$ (5)
- The poles of Eq (5) are identical to the spin flip excitation energies
- $\Delta E_{\uparrow\downarrow}(k,q) = \varepsilon(k+q) - \varepsilon(k) + 2\,U\,m$

- They describe transitions between the two spin bands



- yielding the exchange splitting
- $\Delta E_{ex} = 2\ U\ m$ (6)
- The exchange splitting is temperature dependent.

metal	$m(T=0)$	$\Delta\ E_{ex}\ (T=0)$	T_C (exp. result)	T_C (theoret. result)
Fe	2.22 μ_B	2 eV	1043 K	1320 K
Ni	0.56 μ_B	0.35 eV	631 K	780K
Co	1.7 μ_B	1.5 eV	1388 K	1280K

Table 1: Experimental and theoretical values for magnetic properties of ferromagnetic metals

Evaluation

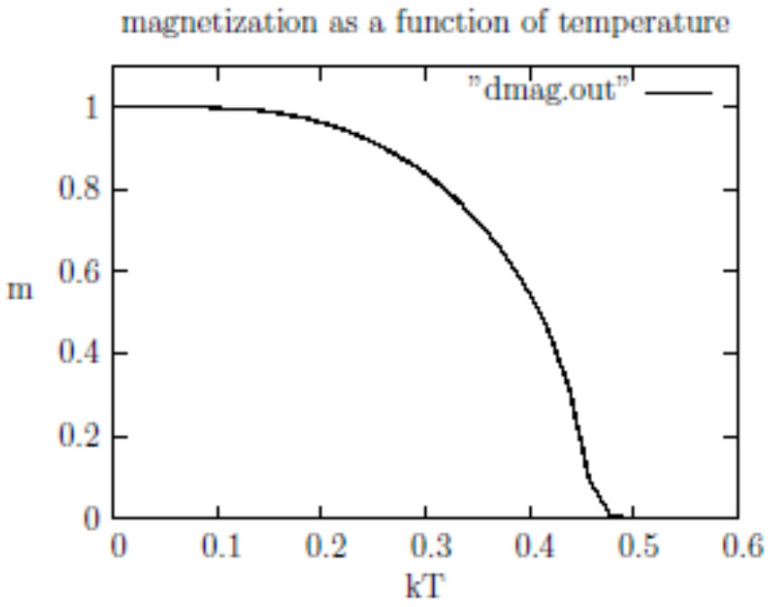
- The particle numbers $n_\uparrow$ and $n_\downarrow$ are calculated from the free Bloch density of states of the non-interacting particle system, i.e.
- $n_\sigma = \int_{-\infty}^{\mu+2\,k_B T} dE\ f_-(E,T)\ \rho_0\ (E - U\, n_{-\sigma})$ (7)
- model density of states:

$$\rho_0(x) = \begin{cases} 1/W \text{ falls } -W/2 \leq x \leq +W/2 \\ 0 \quad \text{sonst} \end{cases}$$

Mit $\mu \approx \varepsilon_F + \frac{1}{2}$ Un folgt dann aus (8.2.21)

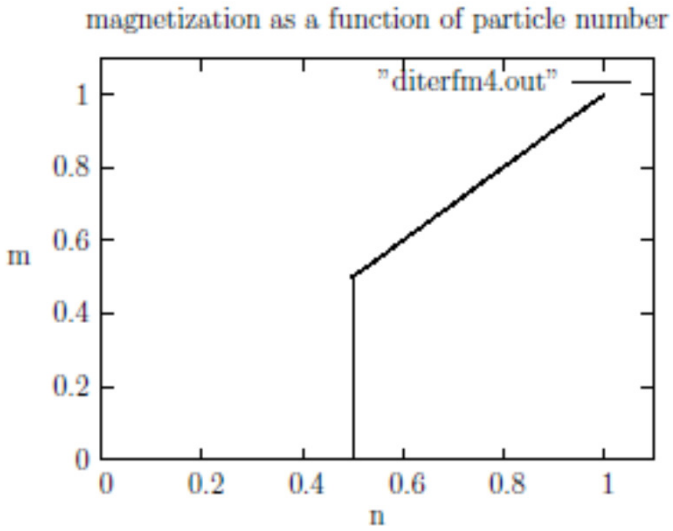
(5) Results

magnetization $m(T, n = const)$.



- The plot $m(T)$ describes the phase transition in a qualitatively correct manner. However, in the vicinity of T_C deviations from the expected results are observed.
- Evaluating the expression for the magnetization in the limit $T \rightarrow T_C$ yields the critical behavior
- $m = \gamma \left(\frac{T_C}{T} - 1\right)^{\beta}$
- $\beta = \frac{1}{2}$ (8)
- The critical exponent of the order parameter in Eq (8) is typical for molecular field approximations.

magnetization $m\ (T = 0, n)$



- The Curie temperature T_C depends on the strength of the ferromagnetic coupling. In the strong coupling limit one obtains
- $k_B\, T_C \;\cong\; \frac{1}{4}\; U$ (9)
- Eq (9) qualitatively agrees with experimental results.

(6) Conclusions and Outlook

- Using the Hubbard Hamiltonian the exchange splitting between the ↑ and ↓ density of states is calculated within an RPA approximation.
- The magnetization $m\ (T, n)$ describes the phase transition in a qualitatively correct manner.
- Ferromagnetic solutions are only obtained for band fillings $n\ \geq 0.5$.
- The dependence of the Curie temperature T_C on the intraatomic Coulomb interaction U qualitatively agrees with experimental results.

- Alternatively the free Bloch density of states of Eq (7) above could also be obtained from a $T = 0K$ band structure calculation of the paramagnetic metal. In the paramagnetic phase the Stoner energies turn out to be identical to renormalized Bloch energies of the form
- $E\,(k) = \varepsilon\,(k) + \frac{1}{2}\,U\,n$
- that include all interactions not covered by the Hubbard Hamiltonian. With these more realistic input parameters Eq (7) may then be reevaluated to obtain improved results for the magnetization $m\,(T, n)$.