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Department of Physics
University of Zurich
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Abstract

Contents

Chapter 1

Charge Order

1.1 Peierl Transition

1.2 From Causality to Kramer-Kronig relation

Looking at a causal function $\tilde{\chi}(t)$, we can split it, like every analytical function, in an even $\chi_{even}(t)$ and an odd $\chi_{odd}(t)$ part.

$$\tilde{\chi}(t) = \begin{cases} 0 & t < t_0 \\ \chi(t) & t > t_0 \end{cases}$$

$$\tilde{\chi}(t) = \frac{\tilde{\chi}(t) + \tilde{\chi}(-t)}{2} + \frac{\tilde{\chi}(t) - \tilde{\chi}(-t)}{2} = \chi_{even}(t) + \chi_{odd}(t) \tag{1.1}$$

Multiplying the even part of this function with the signum function yields,

$$\text{sign}(t) \cdot \chi_{even} = \text{sign}(t) \cdot \left\{ \frac{\tilde{\chi}(t)}{2} + \frac{\tilde{\chi}(-t)}{2} \right\} = \frac{\tilde{\chi}(t)}{2} - \frac{\tilde{\chi}(t)}{2} = \chi_{odd}(t) \tag{1.2}$$

Using this relation to replace $\chi_{odd}(t)$ in Eq. 1.1 .

$$\tilde{\chi}(t) = \chi_{eve} + \chi_{odd} = (1 + \text{sign}(t)) \cdot \chi_{even}(t) = \sigma(t) \cdot \chi_{even}(t) \tag{1.3}$$

Second Quantization: Free Electron Gas

$k_F^3 = 3\pi^2 n$

$E_0 = \frac{3}{5} N epsilon_F$

Bohr Radius: $a_0 = \frac{\hbar}{me^2}$

$$\frac{3\pi^2}{k_F^3} = \frac{1}{n} = \frac{V}{N} = \frac{4\pi}{3}\left(r_S a_0\right)^3 \quad \Rightarrow \quad r_S = \left(\frac{9\pi}{4}\right)^{1/3} \frac{1}{a_0 k_F}$$

$$\frac{E_0}{N} = \frac{2.21}{r_S^2}\frac{e^2}{2a_0}$$

Electron Interaction

$$\frac{E_1}{N} = \frac{\langle FS| V_{el-el} |FS\rangle}{N} = -\frac{e^2}{2}$$

Chapter 2

Magnetism

2.1 Ferromagnetism

2.1.1 $\mathbf{H_2}$ Molecule

Wave Function Considerations

$$\Psi^{Total}(2 \text{ Electrons}) \rightarrow \text{Antisymmetric} \tag{2.1}$$

$$\Psi^{Total}(\vec{r}_1, \vec{r}_2) = -\Psi^{Total}(\vec{r}_2, \vec{r}_1) \tag{2.2}$$

$$\Psi_A = \psi_\alpha(\vec{r}_1)\psi_\beta(\vec{r}_2) - \psi_\alpha(\vec{r}_2)\psi_\beta(\vec{r}_1) \tag{2.3}$$

$$\Psi_S = \psi_\alpha(\vec{r}_1)\psi_\beta(\vec{r}_2) + \psi_\alpha(\vec{r}_2)\psi_\beta(\vec{r}_1) \tag{2.4}$$

Consider now spin wave function:

$$\chi_S = \chi_{Symmetric} = \begin{cases} |\uparrow_\alpha\downarrow_\beta\rangle & |1,1\rangle \\ (|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)/\sqrt{2} & |1,0\rangle \\ |\downarrow_\alpha\uparrow_\beta\rangle & |1,-1\rangle \end{cases} \tag{2.5}$$

$$\chi_A = \chi_{Antisymmetric} = (|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)/\sqrt{2} \quad |0,0\rangle \tag{2.6}$$

Where to the χ_S is refered to as **Triplet state** and to the wave function χ_A is refered to as textbfSinglet state.

Quantum mechanical Spin-Operators

Recalling that $\hat{S}^2|S,m\rangle = S(S+1)|S,m\rangle$ we get for the eigenvalues of $\hat{S}^2_\alpha$ and $\hat{S}^2_\beta$

$$\begin{aligned} \hat{S}^2_\alpha|S_\alpha,m\rangle &= S_\alpha(S_\alpha+1)|S_\alpha,m\rangle &= 3/4 \quad (2.7)\\ \hat{S}^2_\beta|S_\beta,m\rangle &= S_\beta(S_\beta+1)|S_\beta,m\rangle &= 3/4 \quad (2.8)\end{aligned}$$

$$\hat{S} \;=\; \hat{S}_\alpha + \hat{S}_\beta \quad\Rightarrow\quad \hat{S}^2 \;=\; \hat{S}^2_\alpha + \hat{S}^2_\beta + 2\hat{S}_\alpha\hat{S}_\beta \quad\Rightarrow\quad \hat{S}_\alpha\cdot\hat{S}_\beta \;=\; \frac{\hat{S}^2 - \hat{S}^2_\alpha - \hat{S}^2_\beta}{2} \tag{2.9}$$

Calculating $\langle\hat{S}_\alpha\cdot\hat{S}_\beta\rangle$ leads to $1/4$ for χ_S and $-3/4$ for the χ_A case.

Consider weak Coulomb interaction

$$H \;=\; H_{\text{signel-H}} \;+\; H_{\text{int}} \;=\; H_0 \;+\; H_{\text{int}} \tag{2.10}$$

Where the interaction Hamiltonian H_{int} inlcudes the proton-proton, electron-electron, proton 1 - electron 2 and electron 1 - proton 2 interactions.

$$H_{int} \;=\; \frac{e^2}{d_{pp}} \;+\; \frac{e^2}{d_{ee}} \;-\; \frac{e^2}{d_{ep}} \;-\; \frac{e^2}{d_{pe}} \tag{2.11}$$

Here d_{pp} stands for the proton-proton distance, d_{ee} for the electron-electron distance. Furthermore contains $H_{\text{single-H}}$ both Hamiltonians of the single hydrogen atoms

$$H_{\text{single-H}} \;=\; H_{H_1} \;+\; H_{H_2} \;=\; \frac{\hbar}{2m}\left(\nabla^2_\alpha + \nabla^2_\beta\right) \;-\; \left(\frac{e^2}{d_{p_\alpha e_\alpha}} + \frac{e^2}{d_{p_\beta e_\beta}}\right) \tag{2.12}$$

$$E_+ \;=\; E_S \;=\; \langle\Psi_S|H_{\text{int}}|\Psi_S\rangle \;=\; \int(\psi_\alpha\,\psi_\beta + \psi_\beta\,\psi_\alpha)^* H_{\text{int}}(\psi_\alpha\,\psi_\beta + \psi_\beta\,\psi_\alpha)d^3r \tag{2.13}$$

$$E_- \;=\; E_A \;=\; \langle\Psi_S|H_{\text{int}}|\Psi_S\rangle \;=\; \int(\psi_\alpha\,\psi_\beta - \psi_\beta\,\psi_\alpha)^* H_{\text{int}}(\psi_\alpha\,\psi_\beta - \psi_\beta\,\psi_\alpha)d^3r \tag{2.14}$$

By defining $C \equiv C_1 + C_2$ and $J \equiv J_1 + J_2$ one can write the the two energies as

$$E_{\pm} \ = \ C \pm J \tag{2.15}$$

Furthermore for the difference of the singlett- and triplett energy we get

$$E_+ - E_- \ = \ 2J \int \psi^*_\alpha \psi^*_\beta H_{\text{int}} \psi_\alpha \psi_\beta d^3r \tag{2.16}$$

From this equatoin we can associate the introduced variable J as the **Exchange Integral**.

$$J \ = \ \frac{E_+ - E_-}{2} \ = \ \int \psi^*_\alpha \psi^*_\beta H_{\text{int}} \psi_\alpha \psi_\beta d^3r \tag{2.17}$$

What is $\mathbf{H^{Spin}}_{\mathbf{int}}$

$$E_{\pm} \ = \ C \pm J \ = \ C + J/2 + 2J + \cdot\rangle \hat{S}_\alpha \cdot \hat{S}_\beta \langle \ = \ \text{constant} + 2J\rangle \hat{S}_\alpha \cdot \hat{S}_\beta\rangle \tag{2.18}$$

The constant contribution to the energies $E_\pm$ can be neglected since absolute energies values arbitrary. The interesting term for us is the second one on the right-most side. It gives us a quantitative measure of how large the energy difference between the two spin configurations is

$$\Rightarrow \ H^{\text{Spin}}_{\text{int}} \ = \ -2J\hat{S}_\alpha \cdot \hat{S}_\beta \qquad \begin{cases} J > 0 & \Rightarrow \quad E_S > E_A \\ J < 0 & \Rightarrow \quad E_A < E_S \end{cases} \tag{2.19}$$

From the upper formula we see that J us if χ_S or χ_A is prefered. Therefore it can be seen as an indication if ferro- or antiferromagnetism is present in a material.

Ferromagnetism

$$\begin{aligned} H \ &= \ -\sum_{ij} J_{ij} \vec{S}_i \cdot \vec{S}_j \ + \ g\mu_B \cdot \sum_j \vec{S}_j \cdot \vec{B} \\ &= \ -\sum_j \sum_i j_{ij} \vec{S}_i \cdot \vec{S}_j \ + \ g\mu_B \sum_j \vec{S}_j \cdot \vec{B} \\ &= \ g\mu_B \sum_j \vec{S}_j \cdot (\underbrace{\vec{B}_{mf}}_{\text{interal}} \ + \ \underbrace{\vec{B}}_{\text{external}}) \end{aligned} \tag{2.20}$$

Using a mean field approximation we rewrite the interaction from all spins on $\vec{S}_j$ from the first term as with a mean magnetic field $\vec{B}_{mf}$ wheresa we dfined $\vec{B}_{mf} \equiv -2/g\mu_B \sum_i J_{ij} \vec{S}_i$.

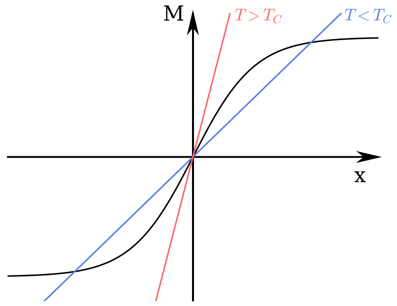

Figure 2.1: Illustration of the grafical solution of 2.22. the straight lines refer to different values of T.

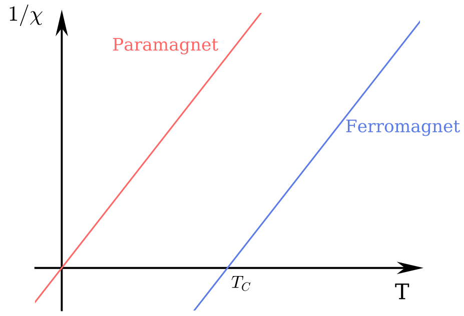

Figure 2.2: Illustration of susceptibility χ of a Para- and Ferromagnet.

Conjecture

By making an educated guess one could assume, that the mean magnetic field $\vec{B}_{mf}$ can be approximated macroscopicaly with the following expression.

$$\vec{B}_{mf} \simeq \lambda \cdot \vec{M} \tag{2.21}$$

Solution

Solution can be adapted from the results about paramagnetism we gained last week. By focusing on the case $\vec{B} = 0$ we get

$$M \simeq N\mu_B \tanh(x) \quad \text{with} \quad x = \frac{\mu_B}{k_B T}(\vec{B} + \lambda\vec{M}) \tag{2.22}$$

Since the argument of the tangent hyperbolicus depends also on the magnetisation $\vec{M}$ we have a implicit equation. A solution of this equation is illustrated in **??** as the crossing point between the hyperbolic tangent and the straight line. In this graph it is also visible, that above a certain Temperature $T > T_C$ there only exists one solution for of the implicit equation which can be associated with the paramagnetic phase of the material. On the other hand for $T < T_C$ we see that there are exists multiple solution of 2.22 which is in accordance with the magnetisation curve of a ferromagnet. We can determine the Transition temperature T_C by comparing the slopes of the two curves at the origin

$$\frac{d}{dx} N\mu_B \tanh(x) = \frac{d}{dx}\frac{k_B T}{\mu_B \lambda} x \quad \Rightarrow \quad T_C = \frac{\lambda N \mu_B^2}{k_B} = \lambda \cdot C \tag{2.23}$$

Looking at the limit $x \ll 1$

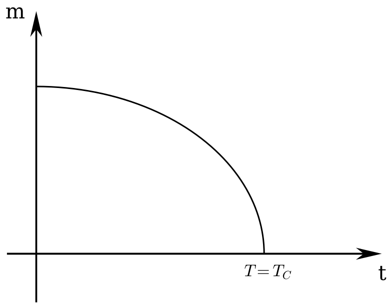

Figure 2.3: Temperature dependence of magnetisation.

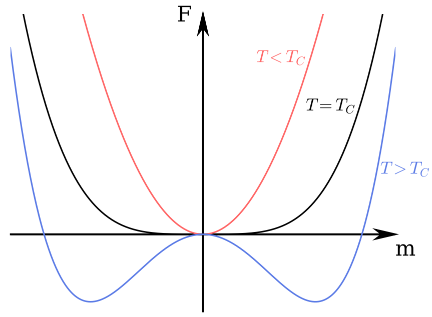

Figure 2.4: Free Energy dependence on the order parameter m for the 3 cases $T < T_C$, $T = T_C$ and $T > T_C$.

$$\left.\begin{array}{lcr} M & = & CB/T \\ \chi & \equiv & M/B \;=\; C/T \end{array}\right\} \rightarrow \begin{array}{lcl} M & = & C\frac{B+\lambda M}{T} \\ \chi & \equiv & \frac{C}{T} + \frac{\lambda}{T}\chi \end{array} \Rightarrow \chi = \frac{C}{T-\lambda C} = \frac{C}{T-T_C}$$

Checking the magnetisation $M(T)$ at zero field $\vec{B} = 0$. Using 2.22 with zero field and the definitinos $m = M/N\mu_B$ and $t = k_B T/N\mu_B^2\lambda = T/T_C$ we get

$$m \;=\; \tanh\left(\frac{m}{t}\right) \tag{2.24}$$

Landau Theory

According to the Landau theory of phase transisiton the free energy F can be expressed

$$F \;=\; F_0 \;+\; a(T)m^2 \;+\; bm^4 + ... \tag{2.25}$$

Were the parameter a and b has to meet the conditions

$$a(T) \;=\; a_0(T - T_C) \quad \text{and} \quad b > 0 \tag{2.26}$$

We find the thermodynamical state of our system by minimizing the free energy

$$\frac{dF}{dm} \;=\; m(2a(T) \;+\; 4bm^2) \;=\; 0 \quad \Rightarrow \quad m \;=\; \left\{\begin{array}{c} 0 \\ \pm\sqrt{\frac{a_0(T-T_C)}{2b}} \end{array}\right. \tag{2.27}$$

2.1.2 Exchange Interaction J

Analog to the susceptibility of ferromagnets $\chi_{FM} = C/(T - T_C)$, we can define the susceptibility for anti-ferromagnets

$$\chi_{AFM} = \frac{C}{T + T_N} \tag{2.28}$$

Where we refer to the Transition Temperature T_N as Neel-Temperature.

2.1.3 Ferromagnetic Magnons

Consider a linear FM chain $|\text{FM}\rangle = |\uparrow\uparrow\uparrow \; ... \rangle$. Applying the latter operator s_j^- onto this expression leads to

$$|j\rangle = s_j^- |\text{FM}\rangle = |\uparrow\uparrow \; ... \uparrow \underbrace{\downarrow}_{j} \uparrow \; ... \rangle \tag{2.29}$$

Defining

$$|q\rangle = \frac{1}{\sqrt{N}} \sum_j e^{iqR_j} |j\rangle \tag{2.30}$$

The Hamilton is given as

$$\begin{aligned} H &= -\sum_{ij} J_{ij} \hat{S}_i \cdot \hat{S}_j = -2J \sum_i \hat{S}_i \cdot \hat{S}_{i+1} \\ &= -2J \sum_i \left\{ \hat{S}_i^z \hat{S}_{i+1}^z + \frac{1}{2} \left[\hat{S}_i^+ \hat{S}_{i+1}^- + \hat{S}_i^- \hat{S}_{i+1}^+ \right] \right\} \end{aligned} \tag{2.31}$$

By taking only nearest neighbour interactions into account we get the The second equality sign holds if we only take neares neighbour interactions into account. To get the final expression we used the substitution

$$\hat{S}^2 = \hat{S}^{z^2} + \frac{1}{2} \left[\hat{S}_i^+ \hat{S}_{i+1}^- + \hat{S}_i^- \hat{S}_{i+1}^+ \right] \tag{2.32}$$

$$H|\text{FM}\rangle = -2JNS^2 |\text{FM}\rangle = E_0 |\text{FM}\rangle \tag{2.33}$$

$$H|j\rangle = -2J \left\{ (N-4) S^2 |j\rangle + S \left[|j+1\rangle + |j-1\rangle \right] \right\} \tag{2.34}$$

$$
\begin{aligned}
H|q\rangle &= \frac{1}{\sqrt{N}}\sum_j e^{iqR_j}\left\{NS^2|j\rangle \;-\; 2S^2|j\rangle \;+\; S|j+1\rangle \;+\; S|j-1\rangle\right\} \\
&= -2JNS^2|q\rangle - 2J\left\{-2S^2 \;+\; \left(e^{iqa}+e^{-iqa}\right)\right\}|q\rangle \\
&= E_0|q\rangle \;+\; 2JS\left\{1-\cos(qa)\right\}|q\rangle \qquad (2.35)
\end{aligned}
$$

Since we are consindering an infinit long 1D chain of spin states we can rewrite the expression

$$
H|q\rangle = E_0|q\rangle + 2JS\left\{2-2\cos(qa)\right\}|q\rangle \qquad (2.36)
$$

which leads to

$$
H|q\rangle = E(q)|q\rangle \qquad \text{with} \qquad E(q) \simeq E_0 + 2JS(2-2\cos(qa)) \qquad (2.37)
$$

This is the dispersion relation for ferromagnets. For anti-ferromagnets we have a similar relation (not derived)

$$
\hbar\omega = 2J|\sin(qa)| \qquad (2.38)
$$

Bibliography