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Abstract

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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.

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


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

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

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

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

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

Second Quantization: Free Electron Gas

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

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

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

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

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

Electron Interaction

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

Chapter 2

Magnetism

2.1 Paramagnetism

Magnetic Moment

insert picture - magnetic moment

If \vec{A} is the area inside the loop and I the current, the magnetic moment can be written as

$$\vec{\mu} = I\vec{A} \quad (2.1)$$

Example: Hydrogen Atom

insert picture - hydrogen atom and orbiting electron

The magnetic moment of a hydrogen atom can be described semi-classically by assuming the electron to be on a fixed trajectory orbiting the hydrogen nucleus with constant radius r and velocity v . The current I produced by the moving electron can be written as $I = -e/\tau$ with the orbital period $\tau = 2\pi r/v$. For the loop area we use the formula $A = \pi r^2$. This leads the magnetic moment to be

$$\mu = \frac{-ev\pi r^2}{2\pi r} = \frac{-evr}{2} = \frac{-emvr}{2m} \quad (2.2)$$

We can identify the classical definition of the angular momentum $\vec{l} = \vec{r} \times m\vec{v}$ in the numerator. Taking the quantisation of angular momentum $|\hat{l}| = n\hbar$ in quantum mechanics into account we can rewrite expression 2.2 for $n = 1$

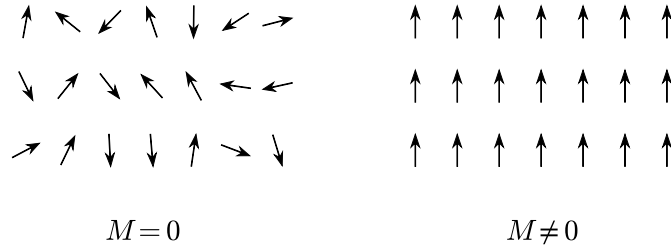


Figure 2.1: hohohoh

$$\mu \simeq \frac{-e\hbar}{2m} \equiv -\mu_B \quad (2.3)$$

Which we define as the Bohr magneton μ_B .

Magnetic Moment of Atoms

The total angular momentum in an atom is given as the sum of total orbital angular Momentum \hat{L} and total spin angular momentum \hat{S}

$$\hat{J} \simeq \hat{L} + \hat{S} \quad (2.4)$$

Magnetisation

Considering a solid with N atoms each having a magnetic moment $\vec{\mu}$. We define the magnetization as

$$\vec{M} \equiv \frac{\text{Magnetic moment}}{\text{Volume}} \quad (2.5)$$

Magnetic Moment in a \vec{B} -Field

From classical electrodynamics we know that the potential energy E of a magnetic moment $\vec{\mu}$ in a magnetic field \vec{B} is described as

$$E = -\vec{\mu} \cdot \vec{B} \quad (2.6)$$

To get a feeling for the order of magnitudes of magnetic energy of atomic scale we

$$\mu_B \times 1\text{Tesla} \simeq 0.05\text{ meV}$$

This is comparable to the energy one has to put into a system to increase its temperature by 1 K ($k_B \cdot 1\text{ K} \simeq 0.084\text{ meV}$).

Magnetic susceptibility

$$\chi \simeq \frac{\mu_0 \vec{M}}{\vec{B}} \quad (2.7)$$

We can look at the magnetic susceptibility χ as response function. χ describes the response of the system \vec{M} when exposed to an external changing field \vec{B} . To simplify things in the calculations we will make the following constraints on \vec{B} .

$$\begin{aligned} \vec{B} \text{ is static} &\Rightarrow \text{no time dependence} \\ \vec{B} \text{ is homogeneous} &\Rightarrow \text{no dependence on } \vec{r} \end{aligned}$$

The definition of the susceptibility allows us now to classify materials depending on how they respond to an external magnetic field. We call materials to be *paramagnetic* if they align their spin parallel to the applied \vec{B} -Field. This is the case if $\chi > 0$. On the contrary we refer to materials as *diamagnetic* if their inner magnetic moments align anti-parallel in respect to an applied field \vec{B} . This results in a negative value for the susceptibility $\chi < 0$.

In reality, the response of systems is composed of multiple different responses which can have different origins.

$$\chi_{total} \simeq \chi_{paramagnetic} + \chi_{diamagnetic} + \dots \quad (2.8)$$

Paramagnetism and diamagnetism can also have different origins. For example:

$$\begin{aligned} \chi_{paramagnetic} &\simeq \chi_{Langevin} + \chi_{Van Vleck} + \chi_{Pauli} + \dots \\ \chi_{diamagnetic} &\simeq \chi_{electronic} + \chi_{superconductivity} + \dots \end{aligned}$$

2.2 Ferromagnetism

2.2.1 H₂ Molecule

Wave Function Considerations

$$\Psi^{Total}(2 \text{ Electrons}) \rightarrow \text{Antisymmetric} \quad (2.9)$$

$$\Psi^{Total}(\vec{r}_1, \vec{r}_2) = -\Psi^{Total}(\vec{r}_2, \vec{r}_1) \quad (2.10)$$

$$\Psi_A = \psi_\alpha(\vec{r}_1)\psi_\beta(\vec{r}_2) - \psi_\alpha(\vec{r}_2)\psi_\beta(\vec{r}_1) \quad (2.11)$$

$$\Psi_S = \psi_\alpha(\vec{r}_1)\psi_\beta(\vec{r}_2) + \psi_\alpha(\vec{r}_2)\psi_\beta(\vec{r}_1) \quad (2.12)$$

Consider now spin wave function:

$$\chi_S = \chi_{Symmetric} = \begin{cases} |\uparrow_\alpha \downarrow_\beta\rangle & |1, 1\rangle \\ (|\uparrow \downarrow\rangle + |\downarrow \uparrow\rangle) / \sqrt{2} & |1, 0\rangle \\ |\downarrow_\alpha \uparrow_\beta\rangle & |1, -1\rangle \end{cases} \quad (2.13)$$

$$\chi_A = \chi_{Antisymmetric} = (|\uparrow \downarrow\rangle - |\downarrow \uparrow\rangle) / \sqrt{2} \quad |0, 0\rangle \quad (2.14)$$

Where to the χ_S is referred to as **Triplet state** and to the wave function χ_A is referred to as **Singlet 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}_α^2 and \hat{S}_β^2

$$\hat{S}_\alpha^2|S_\alpha, m\rangle = S_\alpha(S_\alpha + 1)|S_\alpha, m\rangle = 3/4 \quad (2.15)$$

$$\hat{S}_\beta^2|S_\beta, m\rangle = S_\beta(S_\beta + 1)|S_\beta, m\rangle = 3/4 \quad (2.16)$$

$$\hat{S} = \hat{S}_\alpha + \hat{S}_\beta \Rightarrow \hat{S}^2 = \hat{S}_\alpha^2 + \hat{S}_\beta^2 + 2\hat{S}_\alpha \hat{S}_\beta \Rightarrow \hat{S}_\alpha \cdot \hat{S}_\beta = \frac{\hat{S}^2 - \hat{S}_\alpha^2 - \hat{S}_\beta^2}{2} \quad (2.17)$$

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

$$H = H_{\text{signal-H}} + H_{\text{int}} = H_0 + H_{\text{int}} \quad (2.18)$$

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

$$H_{\text{int}} = \frac{e^2}{d_{pp}} + \frac{e^2}{d_{ee}} - \frac{e^2}{d_{ep}} - \frac{e^2}{d_{pe}} \quad (2.19)$$

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

$$H_{\text{single-H}} = H_{H_1} + H_{H_2} = \frac{\hbar}{2m} (\nabla_\alpha^2 + \nabla_\beta^2) - \left(\frac{e^2}{d_{p_\alpha e_\alpha}} + \frac{e^2}{d_{p_\beta e_\beta}} \right) \quad (2.20)$$

$$E_+ = E_S = \langle \Psi_S | H_{\text{int}} | \Psi_S \rangle = \int (\psi_\alpha \psi_\beta + \psi_\beta \overbrace{\psi_\alpha}^{J_2})^* \overbrace{H_{\text{int}} (\psi_\alpha \psi_\beta + \psi_\beta \psi_\alpha)}^{J_1} d^3r \quad (2.21)$$

$$E_- = E_A = \langle \Psi_S | H_{\text{int}} | \Psi_S \rangle = \int (\psi_\alpha \psi_\beta - \psi_\beta \overbrace{\psi_\alpha}^{J_2})^* \overbrace{H_{\text{int}} (\psi_\alpha \psi_\beta - \psi_\beta \psi_\alpha)}^{J_1} d^3r \quad (2.22)$$

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

$$E_\pm = C \pm J \quad (2.23)$$

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

$$E_+ - E_- = 2J \int \psi_\alpha^* \psi_\beta^* H_{\text{int}} \psi_\alpha \psi_\beta d^3r \quad (2.24)$$

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

$$J = \frac{E_+ - E_-}{2} = \int \psi_\alpha^* \psi_\beta^* H_{\text{int}} \psi_\alpha \psi_\beta d^3r \quad (2.25)$$

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

$$E_{\pm} = C \pm J = C + J/2 + 2J + \langle \hat{S}_{\alpha} \cdot \hat{S}_{\beta} \rangle = \text{constant} + 2J \langle \hat{S}_{\alpha} \cdot \hat{S}_{\beta} \rangle \quad (2.26)$$

The constant contribution to the energies E_{\pm} can be neglected since absolute energies values are 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

$$\Rightarrow H^{\text{Spin}}_{\text{int}} = -2J \hat{S}_{\alpha} \cdot \hat{S}_{\beta} \quad \begin{cases} J > 0 & \Rightarrow E_S > E_A \\ J < 0 & \Rightarrow E_A < E_S \end{cases} \quad (2.27)$$

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

Ferromagnetism

$$\begin{aligned} H &= - \sum_{ij} J_{ij} \vec{S}_i \cdot \vec{S}_j + g\mu_B \cdot \sum_j \vec{S}_j \cdot \vec{B} \\ &= - \sum_j \sum_i J_{ij} \vec{S}_i \cdot \vec{S}_j + g\mu_B \sum_j \vec{S}_j \cdot \vec{B} \\ &= g\mu_B \sum_j \vec{S}_j \cdot \left(\underbrace{\vec{B}_{mf}}_{\text{internal}} + \underbrace{\vec{B}}_{\text{external}} \right) \end{aligned} \quad (2.28)$$

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} whereas we defined $\vec{B}_{mf} \equiv -2/g\mu_B \sum_i J_{ij} \vec{S}_i$.

Conjecture

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

$$\vec{B}_{mf} \simeq \lambda \cdot \vec{M} \quad (2.29)$$

Solution

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

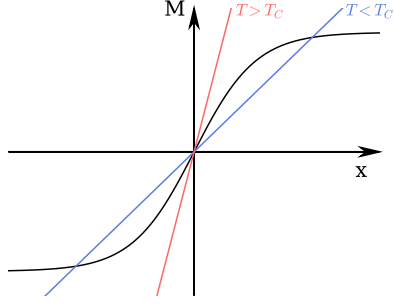


Figure 2.2: Illustration of the graphical solution of 2.30. the straight lines refer to different values of T .

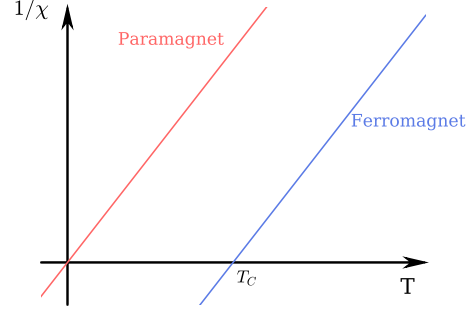


Figure 2.3: Illustration of susceptibility χ of a Para- and Ferromagnet.

$$M \simeq N\mu_B \tanh(x) \quad \text{with} \quad x = \frac{\mu_B}{k_B T}(\vec{B} + \lambda \vec{M}) \quad (2.30)$$

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 2.30 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

$$\frac{d}{dx} N\mu_B \tanh(x) = \frac{d}{dx} \frac{k_B T}{\mu_B \lambda} x \Rightarrow T_C = \frac{\lambda N \mu_B^2}{k_B} = \lambda \cdot C \quad (2.31)$$

Looking at the limit $x \ll 1$

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

Checking the magnetisation $M(T)$ at zero field $\vec{B} = 0$. Using 2.30 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

$$m = \tanh\left(\frac{m}{t}\right) \quad (2.32)$$

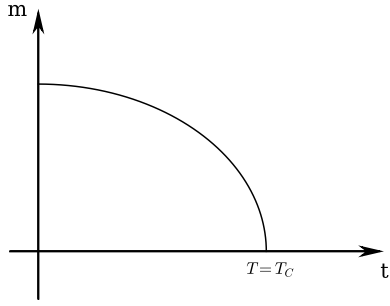


Figure 2.4: Temperature dependence of magnetisation.

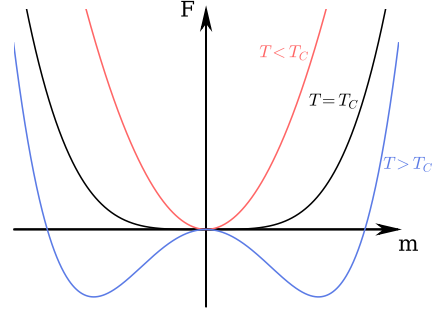


Figure 2.5: Free Energy dependence on the order parameter m for the 3 cases $T < T_C$, $T = T_C$ and $T > T_C$.

Landau Theory

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

$$F = F_0 + a(T)m^2 + bm^4 + \dots \quad (2.33)$$

Were the parameter a and b has to meet the conditions

$$a(T) = a_0(T - T_C) \quad \text{and} \quad b > 0 \quad (2.34)$$

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

$$\frac{dF}{dm} = m(2a(T) + 4bm^2) = 0 \quad \Rightarrow \quad m = \begin{cases} 0 \\ \pm \sqrt{\frac{a_0(T-T_C)}{2b}} \end{cases} \quad (2.35)$$

2.2.2 Exchange Interaction J

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

$$\chi_{AFM} = \frac{C}{T + T_N} \quad (2.36)$$

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

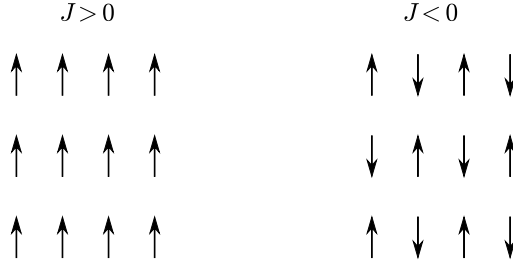


Figure 2.6: hohoho

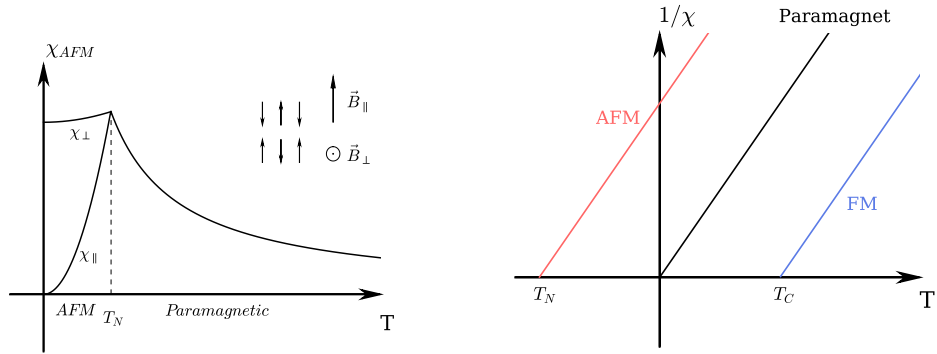


Figure 2.7: Temperature dependence of magneti-

Figure 2.8: Free Energy dependence on the order parameter m for the 3 cases $T < T_C$, $T = T_C$ and $T > T_C$.

2.2.3 Ferromagnetic Magnons

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

$$|j\rangle = s_j^- |\text{FM}\rangle = |\uparrow\uparrow \dots \underbrace{\uparrow\downarrow}_j \uparrow \dots\rangle \quad (2.37)$$

Defining

$$|q\rangle = \frac{1}{\sqrt{N}} \sum_j e^{iqR_j} |j\rangle \quad (2.38)$$

The Hamilton is given as

$$\begin{aligned}
H &= -\sum_{ij} J_{ij} \hat{S}_i \cdot \hat{S}_j = -2J \sum_i \hat{S}_i \cdot \hat{S}_{i+1} \\
&= -2J \sum_i \left\{ \hat{S}_i^z \hat{S}_{i+1}^z + \frac{1}{2} [\hat{S}_i^+ \hat{S}_{i+1}^- + \hat{S}_i^- \hat{S}_{i+1}^+] \right\}
\end{aligned} \tag{2.39}$$

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

$$\hat{S}^2 = \hat{S}^{z^2} + \frac{1}{2} [\hat{S}_i^+ \hat{S}_{i+1}^- + \hat{S}_i^- \hat{S}_{i+1}^+] \tag{2.40}$$

$$H|\text{FM}\rangle = -2JNS^2|\text{FM}\rangle = E_0|\text{FM}\rangle \tag{2.41}$$

$$H|j\rangle = -2J \{ (N-4)S^2|j\rangle + S[|j+1\rangle + |j-1\rangle] \} \tag{2.42}$$

$$\begin{aligned}
H|q\rangle &= \frac{1}{\sqrt{N}} \sum_j e^{iqR_j} \{ NS^2|j\rangle - 2S^2|j\rangle + S|j+1\rangle + S|j-1\rangle \} \\
&= -2JNS^2|q\rangle - 2J \{ -2S^2 + (e^{iqa} + e^{-iqa}) \} |q\rangle \\
&= E_0|q\rangle + 2JS \{ 1 - \cos(qa) \} |q\rangle
\end{aligned} \tag{2.43}$$

Since we are considering an infinite long 1D chain of spin states we can rewrite the expression

$$H|q\rangle = E_0|q\rangle + 2JS \{ 2 - 2\cos(qa) \} |q\rangle \tag{2.44}$$

which leads to

$$H|q\rangle = E(q)|q\rangle \quad \text{with} \quad E(q) \simeq E_0 + 2JS(2 - 2\cos(qa)) \tag{2.45}$$

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

$$\hbar\omega = 2J|\sin(qa)| \tag{2.46}$$

Bibliography