MAGNETIC SUSCEPTIBILITY IN LINEAR RESPONSE

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1 The magnetic moment of the electron

The spin $\vec{S}$ of an electron carries a magnetic moment $\vec{\mu}_s = -g\frac{e}{2mc}\vec{S}$, with Landé factor $g = 2$ resulting from Dirac's equation. In the representation $\vec{S} = (\hbar/2)\vec{\sigma}$ it is $\vec{\mu}_s = -\mu_B\vec{\sigma}$, with Bohr's magneton:

$$\mu_B = \frac{e\hbar}{2mc} = 0.5788 \times 10^{-8}\text{eV/gauss} \tag{1}$$

or $\mu_B = 0.9274 \times 10^{-20}$ erg/gauss. The potential energy of a single spin in a (local) field is $-\vec{\mu}\cdot\vec{B} = \mu_B\vec{\sigma}\cdot\vec{B}$. The Boltzmann factor $e^{-\beta E}$ (E is the energy of the electron) is enhanced if the magnetic moment is aligned with the magnetic induction field (paramagnetism), i.e. the spin is antiparallel.
For an assembly of electrons, one defines the *magnetization density* operators:

$$\vec{m}(\vec{x}) = \sum_i \vec{\mu}_s(\vec{S}_i)\delta_3(\vec{x}-\vec{X}_i) = -\mu_B\sum_{mm'}\psi^\dagger_m(\vec{x})\vec{\sigma}_{mm'}\psi_{m'}(\vec{x}) \tag{2}$$

Exercise: prove that $[m_i(\vec{x}), m_j(\vec{x}')] = i\hbar\delta_3(\vec{x}-\vec{x}')\sum_k \epsilon_{ijk}m_k(\vec{x})$.

2 Spin paramagnetism

We study the gran canonical Hamiltonian $K' = K - \int d^3x\, \vec{m}(\vec{x})\cdot\vec{H}(\vec{x},t)$. According to linear response theory, if the equilibrium magnetization is null, for a weak field it is:

$$m_i(x) = -\frac{1}{\hbar}\int d^4x'\mathcal{D}^{ret}_{ij}(x,x')H_j(x') \tag{3}$$

with the response function $i\mathcal{D}^R_{ij}(x.x') = \theta(t-t')\langle [m_i(x)\,,\,m_j(x')]\rangle$. Since the system at equilibrium is invariant under time-translations, we may shift to ω space:

$$m_i(\vec{x},\omega) = -\frac{1}{\hbar}\int d^3x'\mathcal{D}^{ret}_{ij}(\vec{x},\vec{x}',\omega)H_j(\vec{x}',\omega)$$

Going back to time:

$$m_i(\vec{x},t) = -\frac{1}{\hbar}\int \frac{d\omega}{2\pi}d^3x'\mathcal{D}^R_{ij}(\vec{x},\vec{x}',\omega)H_j(\vec{x}',\omega)e^{-i\omega t}$$

The retarded correlator can be evaluated via the Lehmann representation from the τ - ordered correlator

$$-\mathcal{D}^T_{ij}(\vec{x}\tau,\vec{x}'\tau') = \langle \mathcal{T}\delta m_i(\vec{x}\tau)\delta m_j(\vec{x}'\tau')\rangle,$$

where $\delta m_i(\vec{x}\tau) = m_i(\vec{x}\tau) - \langle m_i(\vec{x})\rangle$. Its expansion in Matsubara frequencies, with *even* frequencies, yields coefficients $\mathcal{D}^T_{ij}(\vec{x},\vec{x}',i\omega_k)$. The retarded correlator is obtained from it by the replacement $i\omega_k$ with $\omega + i\eta$.
In detail:

$$\begin{aligned} -\mathcal{D}^T_{ij}(x,x') &= \mu_B^2\sigma^i_{mm'}\sigma^j_{nn'}\langle \mathcal{T}\psi^\dagger_m(x)\psi_{m'}(x)\psi^\dagger_n(x')\psi_{n'}(x')\rangle - \langle m_i(\vec{x})\rangle\langle m_j(\vec{x}')\rangle \\ &= -\hbar\mu_B^2\sigma^i_{mm'}\sigma^j_{nn'}\Pi_{mm',nn'}(x,x') \end{aligned} \tag{4}$$

where the full polarization of the system at equilibrium appears.

2.1 The polarization

For independent particles the evaluation of the polarization is simple:

$$\Pi_{mm',nn'}(\vec{x},\vec{x}',i\omega_k) = -2\sum_{ab}\langle m'\vec{x}|a\rangle\langle a|m\vec{x}'\rangle\langle n'\vec{x}|b\rangle\langle b|n\vec{x}'\rangle\frac{n_a - n_b}{i\hbar\omega_k - (\epsilon_a - \epsilon_b)}$$

For interacting electrons, the polarization is the sum of diagrams with two electron lines joining in x, (one leaving with spin m and one arriving with spin m') and two lines joining in x' with spin n (outgoing) and n' (ingoing). Since an electron line leaving from x must either return to it or join x', if the system with $\vec{H} = 0$ has Green functions and interactions diagonal in spin, it is:

$$\Pi_{mm',nn'}(x,x') = \delta_{mn'}\delta_{m'n}\Pi_1(x,x') + \delta_{mm'}\delta_{nn'}\Pi_2(x,x')$$

where in Π_1 the points x and x' are joined by two lines, and Π_2 has diagrams where a line closes on x and another closes on x'. All Π_1 diagrams are in

Π^*, but there are also diagrams in Π_2 that belong to Π^* (also for Π^* one can write a decomposition as above). Then:

$$\sigma^i_{mm'}\sigma^j_{nn'}\Pi_{mm',nn'} = \mathrm{tr}(\sigma^i\sigma^j)\Pi_1 + \mathrm{tr}\sigma^i\mathrm{tr}\sigma^j\,\Pi_2 = 2\delta_{ij}\Pi_1$$

where we used the useful relation $\sigma^i\sigma^j = \delta_{ij}I + i\epsilon_{ijk}\sigma_k$ and the fact that Pauli matrices are traceless. In this situation: $\mathcal{D}^R_{ij}(\vec{x},\vec{x}',\omega) = 2\hbar\mu_B^2\delta_{ij}\Pi_1(\vec{x},\vec{x}',\omega + i\eta)$.

2.2 Homogeneous systems

If the system at equilibrium is invariant for space translations, the response function is local in 4D Fourier space: $m_i(k) = -\frac{1}{\hbar}\mathcal{D}^{ret}_{ij}(k)H_i(k)$. The coefficient is the magnetic susceptibility:

$$\chi_{ij}(k) = -\frac{1}{\hbar}\mathcal{D}^{ret}_{ij}(k) \tag{5}$$

and the magnetization density in space time is:

$$m_i(x) = \int \frac{d^3k d\omega}{(2\pi)^4} e^{i\vec{k}\cdot\vec{x}-i\omega t}\chi_{ij}(\vec{k},\omega)H_j(\vec{k},\omega) \tag{6}$$

Moreover, if the field is homogeneous and constant, $H_j(\vec{k}) = H_j\,(2\pi)^4\delta_4(k)$, the resulting magnetization is homogeneous and constant: $m_i = \chi_{ij}H_j$, with

$$\chi_{ij} = -\mu_B^2\sigma^i_{mn}\sigma^j_{m'n'}\Pi_{mn,m'n'}(\vec{k}\to 0) \tag{7}$$

2.3 Ideal electron gas

For the free electron gas, it is

$$\Pi_{mn,m'n'} = (-1/\hbar)(-1)\delta_{mn'}\delta_{m'n}\mathcal{G}^0(x,x')\mathcal{G}^0(x',x) = \frac{1}{2}\delta_{mn'}\delta_{m'n}\Pi^{(0)}(x,x')$$

where $\Pi^{(0)}$ is the polarization bubble diagram. In Fourier space:

$$\Pi^{(0)}(\vec{k},i\omega_n) = -2\int\frac{d^3q}{(2\pi)^3}\frac{n_{\vec{k}+\vec{q}} - n_{\vec{q}}}{i\hbar\omega_n - (\epsilon_{\vec{k}+\vec{q}} - \epsilon_{\vec{q}})} \tag{8}$$

We replace $i\omega_n$ with $\omega + i\eta$ and let $\omega = 0$ without any harm. Then take k to 0:

$$\begin{aligned}\chi_{ij} &= -\mu_B^2\delta_{ij}\lim_{k\to 0}\Pi^{(0)}(k,0) = -2\mu_B^2\delta_{ij}\int\frac{d^3q}{(2\pi)^3}\lim_{k\to 0}\frac{n_{\vec{k}+\vec{q}} - n_{\vec{q}}}{\epsilon_{\vec{k}+\vec{q}} - \epsilon_{\vec{q}}}\\ &= -2\mu_B^2\delta_{ij}\int\frac{d^3q}{(2\pi)^3}\frac{\partial n}{\partial\epsilon}(\vec{q}) = -2\mu_B^2\delta_{ij}\int d\epsilon\rho(\epsilon)\frac{\partial n}{\partial\epsilon}\end{aligned} \tag{9}$$

Therefore $\chi = -\mu_B^2 \int d\epsilon \rho(\epsilon) \frac{\partial n}{\partial \epsilon}$ with limit behaviours: $\chi = \mu_B^2 \rho(\epsilon_F)$ for $T = 0$ (Pauli paramagnetism) and, for large T, $\chi = \frac{\mu_B^2 n}{k_B T}$ (Curie's law) where $n = \int d\epsilon \rho(\epsilon) n_\epsilon$ is the electronic density. The same result could be obtained in few lines by other means.