Quantum magnetism – introductory concepts

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Motivation

- Many exotic quantum phases observed in real quantum magnets, e.g., BEC of magnons, BKT behavior, magnetization plateaus, etc.
- Spin fluctuations are believed to underlie the mechanism behind high-Tc superconductivity in Cuprates
- Tailored quantum magnets possible – can simulate designer Hamiltonians (to a limited extenet)
- Testbed to study several many-body phenomena – specially bosonic phases.
- Possible relevance to quantum information processing / quantum computation (entanglement, decoherence, etc.)

Reference

Quantum Theory of Magnetism, 3rd. Ed. by Robert M. White (Springer 2006)

Origin of magnetic moments

1. Moment due to orbital current density, ***j*** : $$\mathbf{m} = \frac{1}{2c}\int d^3r\,\mathbf{r}\times\mathbf{j}$$

2. Moment due to intrinsic spin (electron): $\mathbf{m} = g\mu_B \mathbf{S}/\hbar, \qquad \mu_B = \dfrac{e\hbar}{2mc}$

g-factor Bohr magneton

For a free electron, Dirac equation gives: *g*=2. Inclusion of radiataive corrections within QED yields a more accurate value

$$g = 2\left\{1 + \frac{\alpha}{2\pi} + \mathcal{O}(\alpha^2\right\}$$

Dirac equation

$$i\hbar\frac{\partial\Psi}{\partial t} = \begin{pmatrix} mc^2 + V & c\sigma\cdot\left(\mathbf{p}+\frac{e}{c}\mathbf{A}\right) \\ c\sigma\cdot\left(\mathbf{p}+\frac{e}{c}\mathbf{A}\right) & -mc^2+V \end{pmatrix} = E\Psi$$

- Ψ is a 4-component Dirac spinor
- Non-relativistic limit -- mc^2 largest energy scale
- Upper 2 components predominantly positive energy components
- But Dirac Hamiltonian mixes the upper and lower components

One can block diagonalize the Dirac Hamiltonian by the Foldy-Wouthuysen transformation.

Expanding in powers of $(mc^2)^{-1}$, we obtain the Hamiltonian for a single electron

$$\begin{aligned}\mathcal{H} \quad &= \quad \frac{1}{2m}\left(\mathbf{p}+\frac{e}{c}\mathbf{A}\right)^2 + V(\mathbf{r}) + \frac{e\hbar}{2mc}\sigma\cdot\mathbf{B} \\ &\quad + \frac{\hbar}{4m^2c^2}\sigma\cdot\nabla V\times\mathbf{p} + \frac{\hbar^2}{8mc^2}\nabla^2 V + \frac{(\mathbf{p}^2)^2}{8m^3c^2} + \ldots\end{aligned}$$

2 terms in the above Hamiltonian involve the electron spin:

$$\mathcal{H}_Z = \frac{e\hbar}{2mc}\sigma\cdot\mathbf{B}$$

Zeeman term

$$\mathcal{H}_{so} = \frac{\hbar}{4m^2c^2}\sigma\cdot\nabla V\times\mathbf{p}$$

spin-orbit interaction

Numerical value of Bohr magneton: $\mu_B = \frac{e\hbar}{2mc} = 5.79\times 10^{-9}\mathrm{e}V/T$

→ Zeeman energy small at realistic magnetic fields.

Bohr-von Leewuen theorem:

Magnetic moment due to orbital elecrton motion cannot be explained by classical statistical mechanics.

Partition function can be made explicitly independent of the vector potential by a simple change of variables.

$$
\begin{aligned}
Z(\mathbf{A}) = \mathrm{Tr} e^{-\beta\mathcal{H}} &= \int \frac{d^N\mathbf{r} d^N\mathbf{p}}{(2\pi\hbar)^{Nd}} e^{-\beta\mathcal{H}(\{\mathbf{p}_i - \frac{q}{c}(\mathbf{A}(\mathbf{r}_i), \mathbf{r}_i\})} \\
&= \int \frac{d^N\mathbf{r} d^N\mathbf{p}}{(2\pi\hbar)^{Nd}} e^{-\beta\mathcal{H}(\{\mathbf{p}_i \mathbf{r}_i\})} = Z(\mathbf{A} = 0)
\end{aligned}
$$

The free energy is independent of $\mathbf{A}$, and hence independent of $\mathbf{B}$

$$
\mathbf{M} = \frac{\partial F}{\partial \mathbf{B}} = 0
$$

OTOH, magnetic moment due to intrinsic spin is correctly described by classical statistical mechanics

$$
\begin{aligned}
Z_{H'berg}(\mathbf{B}) &= \Pi_i \int \frac{d\mathbf{S}_i}{4\pi} e^{\beta J \sum_{\langle i,j\rangle} \mathbf{S}_i \cdot \mathbf{S}_j} e^{\beta g \mu_B \mathbf{B} \cdot \sum_i \mathbf{S}_i} \\
Z_{Ising}(\mathbf{B}) &= \sum_{\{\sigma_i\}} e^{\beta J \sum_{\langle i,j\rangle} \sigma_i \sigma_j} e^{\beta g \mu_B B \sum_i \sigma_i}
\end{aligned}
$$

Atomic magnetism

Hamiltonian for a N-electron atom with nuclear charge Ze

$$\mathcal{H} = \sum_{i=1}^{N}\left[\frac{\mathbf{p}_i^2}{2m} - \frac{Ze^2}{r_i}\right] + \sum_{i<j}^{N}\frac{e^2}{r_{ij}} + \sum_{i=1}^{N}\zeta(r_i)\mathbf{l}_i\cdot\mathbf{s}_i + \sum_i \frac{\mu_B}{\hbar}(\mathbf{l}_i + 2\mathbf{s}_i)\cdot\mathbf{B}$$

Electronic shell configurations: Hund’s rules; periodic table

Crystal field splitting

Degeneracy of (anisotropic) orbitals is lifted by atomic environment in a crystal. Orbitals that minimize Coulomb repulsion with neighboring anions are energetically favored. This can lead to :violation” of Hund’s rule and result in different net spin moment for the same ion in different crystals., e.g., Co^{4+} can carry a net moment $S=1/2$ or $S=5/2$ depending on the crystal structure of the parent compound.

Itinerant magnetism: non-interacting spins

Pauli paramagnetism:

Ignore orbital effects of the applied magnetic field

At $T=0$, $B=0$, electrons fill the Fermi sea with $N_\uparrow = N_\downarrow$

In an external magnetic field, the Zeeman term lifts the degeneracy of the up and dn spins

$$\mathcal{H}_Z = \mu_B B(N_\uparrow - N_\downarrow)$$

The zero-T magnetization density

$$M = -\frac{1}{V}\frac{\partial \mathcal{H}_Z}{\partial B} = \mu_B \frac{(N_\uparrow - N_\downarrow)}{V} \equiv \chi_P B$$

Energy of up/dn spins shifted by $\pm\mu_B B$. This gives

$$\Delta N_\uparrow = -\Delta N_\downarrow = \mu_B B . \frac{1}{2} g(\varepsilon_F) V$$

Hence

$$\boxed{\chi_P = \mu_B^2 g(\varepsilon_F)}$$

Pauli susceptibility: paramagnetic

Landau diamagnetism:

Include orbital contribution *and* finite temperatures

$$\mathcal{H} = \frac{1}{2m}(\mathbf{p} - \frac{e}{c}\mathbf{A})^2 + \mu_B \sigma \cdot \mathbf{B}$$

Quantized energy levels for a charged particle in a uniform field

$$\varepsilon(n, k_z, \sigma) = (n + \frac{1}{2})\hbar\omega_c + \sigma\mu_B B + \frac{\hbar^2 k_z^2}{2m} \qquad \omega_c = \frac{eB}{mc}$$

Cyclotron freq.

$$\Omega(T, V, \mu, B) = -Vk_B T \int d\varepsilon g(\varepsilon) \ln\left[1 + e^{(\mu-\varepsilon)/k_B T}\right]$$

$$g(\varepsilon) = \frac{1}{2\sqrt{2}} \frac{eB\sqrt{m}}{\pi^2\hbar^2 c} \sum_{n=0}^{\infty} \sum_{\sigma=\pm 1} \frac{\Theta(\varepsilon - \varepsilon_{n\sigma})}{\sqrt{\varepsilon - \varepsilon_{n\sigma}}}$$

After some lengthy, but straightforward, algebra we obtain the net susceptibility of free electrons at finite temps

$$\chi = \left(1 - \frac{1}{3}\right) \mu_B^2 \left. \frac{\partial^2 \Omega}{\partial \mu^2} \right|_{B=0}$$

Pauli paramagnetic susceptibility

Landau diamagnetic susceptibility

Itinerant magnetism: interacting spins

Non-interacting electron gas never develops spontaneous long range magnetic order.

Magnetism in solids arise from Coulomb repulsion between electrons.

The Hubbard model:

$$\mathcal{H} = -t \sum_{\langle i,j \rangle \sigma} \left(c^\dagger_{i,\sigma} c_{j,\sigma} + c^\dagger_{j,\sigma} c_{i,\sigma} \right) + U \sum_i n_{i\uparrow} n_{\downarrow} - g\mu_B B \sum_i \frac{(n_{i\uparrow} - n_{i\downarrow})}{2} - \mu \sum_i (n_{i\uparrow} + n_{i\downarrow})$$

- Single band (orbital) model
- Hopping between nearest neighbors
- Long-range Coulomb repulsion approximated by on-site U
- Quantization axis chosen along the magnetic field
- No crystal field effect

The Heisenberg model as the large-U limit if the Hubbard model at half-filling:

- $n_{i\uparrow} + n_{i\downarrow} = 1$
- $t = 0 \Rightarrow$ every site has exactly one electron – massively degenerate ground state
- $t \ll U$, but finite: degeneracy lifted by fluctuations induced by kinetic energy
- 2 antiparallel spins can gain k.e. by virtual tunneling to intermediate state with double occupancy - not possible for parallel spins
- Antiferromagnetism arises naturally from strong Coulomb repulsion
- Extend to an extended lattice to obtain the Heisenberg model

$$\mathcal{H} = J \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j - g\mu_B h_z \sum_i S_i^z$$

Model spin Hamiltonians

Fluctuating magnetic moments at latice sites - charge degrees of freedom “frozen”.

Classical spin systems

Ising model: spins can locally exist in 2 states – up or down

$$S_i = \pm 1, \qquad E = J \sum_{\langle i,j \rangle} S_i S_j$$

XY model: spins are represented by a vector of fixed length in the XY plane

$$S_i = (\cos\theta_i, \sin\theta_i), \qquad E = J \sum_{\langle i,j \rangle} \cos(\theta_i - \theta_j)$$

Heisenberg model: spins are vectors of fixed length on a sphere

$$S_i = (\sin\theta_i \cos\phi_i, \sin\theta_i \sin\phi_i, \cos\theta_i), \qquad E = J \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j$$

Quantum spin systems

Projection of individual spins on the quantization axis takes discrete values

$$S_i^z = -S, -S+1, \ldots, S-1, S$$

Spin operators obey commutation relations

$$[S_i^x, S_i^y] = i\hbar S_i^z$$

Raising and lowering operators defined as

$$S_i^{\pm} = S_i^x \pm i S_i^y$$

$$S_i^{\pm}|S_i^z\rangle = \sqrt{S(S+1) - S_i^z(S_i^z \pm 1)}|S_i^z \pm 1\rangle$$

Quantum Heisenberg model

$$\mathcal{H} = J \sum_{\langle i,j \rangle} \left[\frac{1}{2} \left(S_i^+ S_j^- + S_j^+ S_i^- \right) + S_i^z S_j^z \right]$$

Mean field theory

$$\mathcal{H} = -J\sum_{\langle i,j\rangle}\mathbf{S}_i\cdot\mathbf{S}_j - \gamma\sum_i \mathbf{h}\cdot\mathbf{S} \qquad J>0$$

Assume small fluctuations about mean value

$$\mathbf{S}_i = \mathbf{m}_i + \delta\mathbf{S}_i, \quad \mathbf{m}_i = \langle\mathbf{S}_i\rangle$$

$$\begin{aligned}\mathbf{S}_i\cdot\mathbf{S}_j &= \mathbf{m}_i\cdot\mathbf{m}_j + \mathbf{m}_i\cdot\delta\mathbf{S}_j + \mathbf{m}_j\cdot\delta\mathbf{S}_i + \delta\mathbf{S}_i\cdot\delta\mathbf{S}_j \\ &= -\mathbf{m}_i\cdot\mathbf{m}_j + \mathbf{m}_i\cdot\mathbf{S}_j + \mathbf{m}_j\cdot\mathbf{S}_i + \delta\mathbf{S}_i\cdot\delta\mathbf{S}_j\end{aligned}$$

Neglecting higher order fluctuation terms

$$\begin{aligned}\mathcal{H}^{\mathrm{MF}} &= J\sum_{\langle i,j\rangle}\mathbf{m}_i\cdot\mathbf{m}_j - \sum_i\left(\gamma\mathbf{h}_i + J\sum_j\mathbf{m}_j\right)\cdot\mathbf{S}_i \\ &\equiv E_0 - \gamma\sum_i\mathbf{h}_i^{\mathrm{eff}}\cdot\mathbf{S}_i\end{aligned}$$

where
$$\begin{aligned}E_0 &= J\sum_{\langle i,j\rangle}\mathbf{m}_i\mathbf{m}_j \\ \mathbf{h}_i^{\mathrm{eff}} &= \mathbf{h}_i + \frac{1}{\gamma}J\sum_j\mathbf{m}_j\end{aligned}$$

external field + internal field

Self-consistency requires that the mean local magnetization satisfies the following

$$\mathbf{m}_i = \frac{\mathrm{Tr}\mathbf{S}_i \exp(\gamma \mathbf{h}_i^{eff} \cdot \mathbf{S}_i / k_B T)}{\mathrm{Tr} \exp(\gamma \mathbf{h}_i^{eff} \cdot \mathbf{S}_i / k_B T)}$$

Under the same conditions, the free energy is given by

$$F\{\mathbf{m}_i\} = J \sum_{\langle i,j \rangle} \mathbf{m}_i \cdot \mathbf{m}_j - k_B T \sum_i \ln \mathrm{Tr} \exp\left(\beta\gamma \mathbf{h}_i^{\mathrm{eff}} \cdot \mathbf{S}_i\right)$$

Some commonly used classical models

Ising model: $S_i = \pm 1$

$$m_i = \tanh(\beta\gamma h_i + \beta J z m)$$

$$F\{m_i\} = J \sum_{\langle i,j \rangle} m_i m_j - k_B T \sum_i \ln 2 \cosh\left(\beta\gamma h_i + \beta z J m\right)$$

Ising model: $S_i = -1, 0, +1$

$$m = \frac{2\sinh(\beta\gamma h_i + \beta zJm)}{1 + 2\cosh(\beta\gamma h_i + \beta zJm)}$$

$$F\{m_i\} = J\sum_{\langle i,j\rangle} m_i m_j - k_B T \sum_i \ln\left\{1 + 2\cosh\left(\beta\gamma h_i + \beta zJm\right)\right\}$$

Heisenberg model: $S_i = (\sin\theta_i\cos\phi_i, \sin\theta_i\sin\phi_i, \cos\theta_i)$

$$\begin{aligned} m_i = \langle\cos\theta_i\rangle &= 2\pi\frac{\int_0^{2\pi} d\theta_i \sin\theta_i\cos\theta_i\exp\left\{\beta\cos\theta_i\left(\gamma h_i + zJm\right)\right\}}{\int_0^{2\pi} d\theta_i \sin\theta_i\exp\left\{\beta\cos\theta_i\left(\gamma h_i + zJm\right)\right\}} \\ &= \coth\left(\beta\gamma h_i + \beta zJm\right) - \frac{k_B T}{\gamma h + zJm} \end{aligned}$$

Quantum antiferromagnetic Heisenberg model

$$\mathcal{H} = J\sum_{\langle i,j\rangle} \mathbf{S}_i\cdot\mathbf{S}_j - \gamma\sum_i \mathbf{h}\cdot\mathbf{S} \qquad J>0$$

Assume bipartite lattice – 2 order parameters $\boldsymbol{m}_{\mathbf{A}}$ and $\boldsymbol{m}_{\mathbf{B}}$ sublattice magnetization

Proceed as before – small fluctuations about mean field values of magnetizations

Effective field on each sublattice

$$\mathbf{h}^{eff}_{A,B} = \mathbf{h} + \gamma^{-1} zJ\mathbf{m}_{B,A}$$

For a spin-S Heisenberg model $S_i^z \in \{-S, -S+1, \ldots, +S\}$

$$\mathrm{Tr}\exp(\beta\gamma\mathbf{h}^{eff}_A\cdot\mathbf{S}_i^A) = \frac{\sinh\left(S+\frac{1}{2}\right)\beta\gamma h^{eff}_A}{\sinh\frac{1}{2}\beta\gamma h^{eff}_A}$$

$$\mathbf{m}_A = \beta\gamma\mathbf{h}^{eff}_A SB_S(S\beta\gamma h^{eff}_A)$$

Optimum configuration – canted antiferromagnetic ordering – spin flop