Recall previously introduced Green's functions:

$$G^{Ret}_{AB}(t,t') = \langle\langle A(t), B(t') \rangle\rangle^{Ret} = -i\theta(t-t')\langle [A(t), B(t')]_{-\zeta} \rangle \quad \{\text{We had } \zeta = 1\}$$

$$G^{Adv}_{AB}(t,t') = \langle\langle A(t), B(t') \rangle\rangle^{Adv} = +i\theta(t'-t)\langle [A(t), B(t')]_{-\zeta} \rangle \quad \text{(Advanced Green's function)}$$

$$G^{c}_{AB}(t,t') = \langle\langle A(t), B(t') \rangle\rangle^{c} = -i\langle T_\zeta (A(t), B(t')) \rangle \quad \text{(Causal Green's function)}$$

$$S_{AB}(t,t') = \frac{1}{2\pi}\langle [A(t), B(t')]_{-\zeta} \rangle \quad \text{(Spectral density)}$$

$$\langle A(t) B(t') \rangle, \langle B(t') A(t) \rangle \quad \text{(Correlation functions)}$$

Particularly important was $G^{Ret}_{AB}(t,t')$, because it appears in linear response theory (Kubo formula)

$$\boxed{\Delta A_t = \frac{1}{\hbar}\int_{-\infty}^{\infty} dt' f_{t'} G^{Ret}_{AB}(t,t')}$$

Some important examples:

- time-dependent magnetic field $\vec{B}_t$ (e.g. uniform in space); couples to magnetic moment of the system constituents

$$\vec{m} = \sum_i \vec{m}_i = \mu_B \sum_i \vec{S}_i$$

The perturbation term in the Hamiltonian: $V_t = -\vec{B}_t \vec{m}$

- Reaction of the magnetization to the switched-on magnetic field

$$\vec{M} = \frac{1}{V}\langle \vec{m} \rangle$$

$$M^\beta_t - M^\beta_0 = -\text{const}\,\frac{1}{V}\sum_\alpha \int_{-\infty}^{\infty} dt' B^\alpha_{t'} \underbrace{\langle\langle m^\beta(t), m^\alpha(t') \rangle\rangle}_{\sim \text{ MAGNETIC SUSCEPTIBILITY TENSOR}}$$

{ SOME MORE – EXERCISE CLASS }

We also introduced (and computed in absence of interactions) the one-electron Green's function, where A, B are creation/annihilation operators. Now elaborate a bit more on this.

$$G^\alpha_{\vec{k}\sigma}(E) = \langle\langle a_{\vec{k}\sigma}, a^\dagger_{\vec{k}\sigma} \rangle\rangle^\alpha_E$$

$$\left\{ \begin{array}{ll} a_{\vec{k}\sigma} \longleftrightarrow A & \zeta = -1 \\ a^\dagger_{\vec{k}\sigma} \longleftrightarrow B & \alpha \in \{Ret, Adv, c\} \end{array} \right\}$$

$$G^{Ret/Adv}_{\vec{k}\sigma}(E) = \frac{\hbar}{E - (\epsilon_{\vec{k}\sigma} - \mu) \pm i0^+}$$

singularities $\longleftrightarrow$ excitation energies

Spectral density $S_{\vec{k}\sigma}(E) = \hbar\,\delta(E - (\epsilon_{\vec{k}\sigma} - \mu))$

$$G^{Ret}_{\vec{k}\sigma}(t-t') = -i\,\theta(t-t')\, e^{-\frac{i}{\hbar}(\epsilon_{\vec{k}\sigma}-\mu)(t-t')}$$

Oscillatory behavior with a frequency corresponding to excitation energy

{ For interacting systems this remains valid ; there is additionally a damping factor interpreted as lifetime of quasiparticles }

Interacting systems $G^{\alpha}_{\vec{k}\sigma}(E) = \dfrac{\hbar}{E-(\epsilon_{\vec{k}\sigma}-\mu+\Sigma^{\alpha}_{\sigma}(\vec{k},E))}$

SELF ENERGY

Dyson eq: $G_{\vec{k}\sigma}(E) = G^{(0)}_{\vec{k}\sigma}(E) + \frac{1}{\hbar} G^{(0)}_{\vec{k}\sigma}(E)\Sigma_{\sigma}(\vec{k},E) G_{\vec{k}\sigma}(E)$

$\Sigma$ MUCH EASIER TO CALCULATE THAN $G$ (E.G IN P.T)

{ $\mathrm{Re}\,\Sigma^{\alpha}_{\sigma}(\vec{k},E)$ – modifies the energies of excitations

$\mathrm{Im}\,\Sigma^{\alpha}_{\sigma}(\vec{k},\sigma)$ – related to excitations' lifetimes } (excitations $\leftrightarrow$ quasiparticles)

## Mean-field approximation

General idea: $A, B$ - operators

$$AB = (A-\langle A\rangle)(B-\langle B\rangle) + A\langle B\rangle + \langle A\rangle B - \langle A\rangle\langle B\rangle$$

Approximation: drop $(A-\langle A\rangle)(B-\langle B\rangle)$ - "small fluctuations"

$$AB \longrightarrow A\langle B\rangle + \langle A\rangle B - \langle A\rangle\langle B\rangle$$

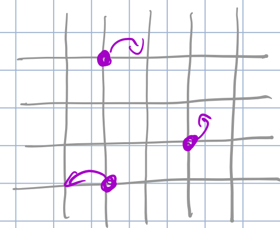
(neglects fluctuations of observables around their thermodynamic averages)

- Very fruitful in many contexts.
- Usually requires additional approximations/knowledge about the system.
- Uncontrolled.

# Example: Electronic ferromagnetism - Stoner theory

Electrons on a lattice $H=\sum_{ij\sigma} T_{ij}\, a^{\dagger}_{i\sigma} a_{j\sigma} + \frac{1}{2}U \sum_{i\sigma} n_{i\sigma} n_{i-\sigma}$ $\quad U>0$

$$\mathcal{H} = H - \mu N = \sum_{ij\sigma} \left(T_{ij} - \mu\delta_{ij}\right) a^{\dagger}_{i\sigma} a_{j\sigma} + \frac{1}{2} U \sum_{i\sigma} n_{i\sigma} n_{i-\sigma}$$



Why might ferromagnetism occur in such a system?

We will first calculate the electronic Green's function starting from real-space (Wannier) representation $G^{\alpha}_{ij\sigma}(E) := \langle\langle a_{i\sigma}\, a^{\dagger}_{j\sigma} \rangle\rangle^{\alpha}_{E}$

Eom: $E\langle\langle A,B\rangle\rangle^{\alpha}_{E} = \hbar \langle [A,B]_{-\varsigma}\rangle + \langle\langle [A,H]_{-}, B \rangle\rangle$ ; $A \to a_{i\sigma}$ $B \to a^{\dagger}_{j\sigma}$

$\Big\{$ We need $[a_{i\sigma}, \mathcal{H}]_{-}$. By direct calculation: $[a_{i\sigma}, \mathcal{H}]_{-} = \sum_{l} (T_{il} - \mu\delta_{il}) a_{l\sigma} + U n_{i-\sigma} n_{i\sigma}$ $\Big\}$

$$E G^{\alpha}_{ij\sigma}(E) = \hbar\delta_{ij} + \sum_{l} T_{il}\, G^{\alpha}_{lj\sigma}(E) - \mu G^{\alpha}_{ij\sigma}(E) + \underbrace{U \langle\langle n_{i-\sigma} a_{i\sigma}, a^{\dagger}_{j\sigma}\rangle\rangle^{\alpha}_{E}}_{\Gamma^{\alpha}_{ij\sigma}(E)}$$

(notation)

Mean-field: $n_{i-\sigma} a_{i\sigma} \longrightarrow n_{i\sigma} \underbrace{\langle a_{i\sigma}\rangle}_{=0} + \underbrace{\langle n_{i-\sigma}\rangle}_{=n_{-\sigma}} a_{i\sigma} - \langle n_{i-\sigma}\rangle \underbrace{\langle a_{i\sigma}\rangle}_{=0}$

(does not depend on $i$)

This simplifies our eom, since $\frac{1}{U}\Gamma^{\alpha}_{ij\sigma}(E) \xrightarrow{MF} \langle n_{-\sigma}\rangle \langle\langle a_{i\sigma}, a^{\dagger}_{j\sigma}\rangle\rangle^{\alpha}_{E} = \langle n_{-\sigma}\rangle G^{\alpha}_{ij\sigma}(E)$

$$\left(E + \mu - U\langle n_{-\sigma}\rangle\right) G^{\alpha}_{ij\sigma}(E) \overset{MF}{=} \hbar\delta_{ij} + \sum_{l} T_{il}\, G^{\alpha}_{lj\sigma}(E)$$

Fourier transform $\Big\{ T_{ij} = \frac{1}{N} \sum_{k} \epsilon_{k}\, e^{ik(R_i - R_j)}$

$$\to \left(E + \mu - U\langle n_{-\sigma}\rangle\right) G^{\alpha}_{k\sigma}(E) = \hbar + \epsilon_{k}\, G_{k\sigma}(E)$$

$$\to G^{Ret/Adv}_{k\sigma}(E) = \frac{\hbar}{E - (\epsilon_{k} - \mu + \underbrace{U\langle n_{-\sigma}\rangle}_{\text{self-energy!}}) \pm i0^{+}}$$

We assumed translational symmetry $\left(\langle n_{i-\sigma}\rangle = \langle n_{-\sigma}\rangle\right)$ but not $\langle n_{-\sigma}\rangle = \langle n_{\sigma}\rangle$

We still do not know $\langle n_{-\sigma}\rangle$...

Proceed along the same line as for the non-interacting case

$$\left\{ \langle B(t')A(t)\rangle = \frac{1}{\hbar}\int dE \frac{S_{AB}(E)}{e^{\beta E}-S_{=-1}} e^{-\frac{i}{\hbar}E(t-t')} \quad (\text{spectral th.}) \right\}$$

$$G^{Ret}_{\vec{k}\sigma}(E) = \int_{-\infty}^{\infty} dE' \frac{S_{\vec{k}\sigma}(E')}{E-E'+i0^+} \implies S_{\vec{k}\sigma}(E) = \hbar\,\delta\big(E-(\epsilon_{\vec{k}}-\mu+U\langle n_{-\sigma}\rangle)\big)$$

With $B \to a^\dagger_{\vec{k}\sigma}$, $A \to a_{\vec{k}\sigma}$ we have

$$\langle a^\dagger_{\vec{k}\sigma}(t')a_{\vec{k}\sigma}(t)\rangle\Big|_{t=t'} = \frac{1}{\hbar}\int_{-\infty}^{\infty} dE\, \frac{\hbar\,\delta(E-(\epsilon_{\vec{k}}-\mu+U\langle n_{-\sigma}\rangle))}{e^{\beta E}+1} =$$

$$= \frac{1}{e^{\beta(\epsilon_{\vec{k}}-\mu+U\langle n_{-\sigma}\rangle)}+1}$$

And so $\langle n_{\vec{k}\sigma}\rangle = \dfrac{1}{e^{\beta(\epsilon_{\vec{k}}-\mu+U\langle n_{-\sigma}\rangle)}+1}$

For simplicity (in performing the integrals):
- Restrict to $T=0$
- Take $\epsilon_{\vec{k}} = \frac{\hbar^2 k^2}{2m}$ (lattice $\to$ continuum)

$$\langle N_\sigma\rangle = \sum_{\vec{k}} \langle n_{\vec{k}\sigma}\rangle \xrightarrow{V\to\infty} \frac{V}{(2\pi)^3}\int d^3k \langle n_{\vec{k}\sigma}\rangle \overset{T=0}{=} \frac{V}{(2\pi)^3}\int d^3k\, \Theta\big(\mu-\epsilon_{\vec{k}}-U\langle n_{-\sigma}\rangle\big) = \left\{\epsilon_{\vec{k}} = \frac{\hbar^2k^2}{2m}\right\} =$$

$$= \frac{V}{2\pi^2}\int_0^\infty dk\, k^2\, \Theta\Big(\mu-\frac{\hbar^2k^2}{2m}-U\langle n_{-\sigma}\rangle\Big) = \frac{V}{6\pi^2}k^3_{F\sigma}$$

with $k_{F\sigma}$ given by $\frac{\hbar^2 k^2_{F\sigma}}{2m} + U\langle n_{-\sigma}\rangle = \mu$

So we have $\langle n_\sigma\rangle = \dfrac{\langle N_\sigma\rangle}{V}$

$$\langle n_\sigma\rangle \overset{\text{notation}}{=} \bar{n}_\sigma$$

$$\begin{cases} (1)\ \bar{n}_\sigma = \frac{1}{6\pi^2}k^3_{F\sigma} \\ (2)\ \frac{\hbar^2k^2_{F\sigma}}{2m} + U\bar{n}_{-\sigma} = \mu \end{cases} \longrightarrow \begin{cases} k^2_{F\sigma} = (6\pi^2\bar{n}_\sigma)^{\frac{2}{3}} \\ \frac{\hbar^2}{2m}(6\pi^2\bar{n}_\sigma)^{\frac{2}{3}} + U\bar{n}_{-\sigma} = \mu \end{cases}$$

Write down an analogous set of equations with $\sigma \to -\sigma$ and subtract

$$\to \frac{\hbar^2}{2m}(6\pi^2)^{\frac{2}{3}}\left(\bar{n}_\sigma^{\frac{2}{3}} - \bar{n}_{-\sigma}^{\frac{2}{3}}\right) + U(\bar{n}_{-\sigma}-\bar{n}_\sigma) = 0$$

Take $\sigma = \uparrow$

$$\bar{n}_\uparrow^{\frac{2}{3}} - \bar{n}_\downarrow^{\frac{2}{3}} = \frac{2mU}{\hbar^2(6\pi^2)^{\frac{2}{3}}}(\bar{n}_\uparrow - \bar{n}_\downarrow)$$

Introduce $\bar{n} := \bar{n}_\uparrow + \bar{n}_\downarrow$ (density)

$$\xi := \frac{\bar{n}_\uparrow - \bar{n}_\downarrow}{\bar{n}} \quad (\sim \text{magnetization})$$

$$\left(\frac{\bar{n}_\uparrow}{\bar{n}}\right)^{\frac{2}{3}} - \left(\frac{\bar{n}_\downarrow}{\bar{n}}\right)^{\frac{2}{3}} = \underbrace{\frac{2mU}{\hbar^2(6\pi^2)^{\frac{2}{3}}}\bar{n}^{-\frac{1}{3}}}_{:=\gamma_0}\xi$$

However:
$$\begin{cases} \dfrac{\bar{n}_\uparrow}{\bar{n}} = \dfrac{1}{2}(\xi+1) \\ \dfrac{\bar{n}_\downarrow}{\bar{n}} = \dfrac{1}{2}(-\xi+1) \end{cases}$$

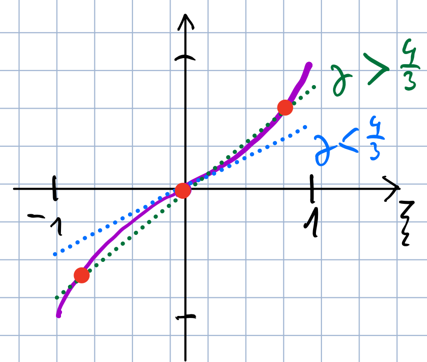
$$\frac{1}{2^{2/3}}\left[(\xi+1)^{\frac{2}{3}} - (1-\xi)^{\frac{2}{3}}\right] = \gamma_0\xi$$

$$\gamma := \gamma_0 2^{\frac{2}{3}}$$

$$(*) \qquad (1+\xi)^{\frac{2}{3}} - (1-\xi)^{\frac{2}{3}} = \gamma\xi \qquad (\xi \in [-1,1])$$

(Equation for $\xi$ !)

- if $\xi$ is a solution, then so is $-\xi$.
- $\xi = 0$ is always a solution.
- $\left[(1+\xi)^{\frac{2}{3}} - (1-\xi)^{\frac{2}{3}}\right]'_{\xi=0} = \frac{4}{3}$
- $\left[(1+\xi)^{\frac{2}{3}} - (1-\xi)^{\frac{2}{3}}\right]_{\xi=\pm 1} = \pm 2$
- $\left[(1+\xi)^{\frac{2}{3}} - (1-\xi)^{\frac{2}{3}}\right]'' > 0 \iff \xi > 0$




There exist solutions with $|\xi| > 0$ for $\gamma > \frac{4}{3}$ (large $U$, small $\bar{n}$)

– spontaneous magnetization (self-energy effect) for $\gamma > \frac{4}{3}$ the solution with $\zeta = 0$ loses thermodynamic stability (we do not show this here)

$\Rightarrow$ Electronic ferromagnetism (due to repulsive interactions + Pauli principle).