Charge density wave order

Many materials undergo phase transitions from an unordered or disordered high temperature phase to an ordered low temperature phase — as an example consider iron magnets.

In this class we will study two kinds of order charge density wave and superconductivity. We start with CDW's.

A charge density wave is a modulation of the electronic charge over the lattice with a characteristic ordering wave vector. Think of a checkerboard and put one density on the red and another on the black. That would be a CDW phase.

How do we calculate such a phase? Imagine adding a field

$$-h = -\sum_j h_j n_j = -\sum_j h_j c_j^\dagger c_j$$

to the Hamiltonian. This will cause a distortion of the density to create a CDW. If the distortion survives as $h \to 0$ the system will spontaneously order. The criterion for this to occur is that the derivative of the density with respect to h diverges as $h \to 0$.

So we start by computing

$$T \left.\frac{d\langle n_i\rangle}{dh_j}\right|_{h=0} = T \frac{d}{dh_j}\left(\mathrm{Tr}\; e^{-\beta H + \beta\sum_k h_k n_k}\, n_i \,\frac{1}{Z(h)}\right)\Bigg|_{h=0}$$

$$Z(h) = \mathrm{Tr}\; e^{-\beta H + \beta\sum_i h_i n_i}$$

We cannot take the derivative of $e^{-\beta H + \beta\sum_i h_i n_i}$ with respect to h because H does not generically commute with $\sum_i h_i n_i$. So we need to go to the interaction picture

$$e^{-\beta H + \beta\sum_i h_i n_i} = e^{-\beta H}\, T_\tau\, e^{+\int_0^\beta h_i n_i(\tau)\, d\tau}$$

with $n_i(\tau) = e^{\tau H} n_i e^{-\tau H}$. Now we can take the derivative.

$$\left.\frac{d Z(h)}{dh_j}\right|_{h=0} = \mathrm{Tr}\; e^{-\beta H}\int_0^\beta n_j(\tau)\, d\tau$$

$$= \mathrm{Tr}\; e^{-\beta H}\int_0^\beta e^{\tau H} n_j e^{-\tau H} = \int_0^\beta d\tau\, \mathrm{Tr}\; \underbrace{e^{-\tau H} e^{-\beta H} e^{\tau H}}_{e^{-\beta H}} n_j$$

$$Z\beta\,\mathrm{Tr}\; e^{-\beta H} n_j = \beta Z\langle n_j\rangle$$

$$\frac{d}{dh_j} Z\langle n_i\rangle = \mathrm{Tr}\; e^{-\beta H}\int_0^\beta d\tau\, n_j(\tau)\, n_i(0) = \int_0^\beta d\tau\; Z\langle n_j(\tau) n_i(0)\rangle$$

So
$$T\frac{d\langle n_i\rangle}{dh_j} = \left[T\int_0^\beta d\tau \underbrace{\left(\langle n_j(\tau) n_i(0)\rangle - \langle n_j\rangle\langle n_i\rangle\right)}_{\text{called the static charge susceptibility}}\right]$$

$$= T\,\chi(R_i - R_j) \quad \text{(translationally invariant system)}$$

Since $\langle n_i \rangle = T \sum_n G_{ii}(i\omega_n)$

$$T\chi(R_i - R_j) = T^2 \sum_n \frac{d}{dh_j} G_i(i\omega_n)$$

recall $G_{ij}(\tau) = -\langle T_\tau c_i(\tau) c_j^\dagger(0) \rangle$

$G_{ij}(i\omega_n) = $ FT of $G_{ij}(\tau)$

Use $GG^{-1}G$ trick to write

$$T\chi(R_i - R_j) = T^2 \sum_n \sum_{j'k} \frac{d}{dh_j}\left(G_{ij'}(i\omega_n)\, G^{-1}_{j'k}(i\omega_n)\, G_{ki}(i\omega_n)\right)$$

or $$T\chi(R_i - R_j) = -T^2 \sum_n \sum_{j'k'} G_{ij'}(i\omega_n)\left(\frac{d}{dh_j} G^{-1}_{j'k}(i\omega_n)\right) G_{ki}(i\omega_n)$$

But $G^{-1}_{j'k}(i\omega_n) = \left(i\omega_n + \mu + h_{j'} - \Sigma_n^{j'j'}\right)\delta_{j'k} - t_{j'k}$

so

$$\frac{d}{dh_j} G^{-1}_{j'k}(i\omega_n) = +\delta_{j'k}\delta_{jj'} - \frac{d\Sigma_n^{j'j'}}{dh_j}\delta_{j'k}$$

and $$T\chi(R_i - R_j) = -T^2 \sum_n \sum_k G_{ik}(i\omega_n) G_{ki}(i\omega_n)\left(\delta_{kj} - \frac{d\Sigma_n^{kk}}{dh_j}\right)$$

$$\boxed{\chi(R_i - R_j) = -T\sum_n G_{ij}(i\omega_n) G_{ji}(i\omega_n) + T\sum_n \sum_k G_{ik}(i\omega_n) G_{ki}(i\omega_n) * \left.\frac{d\Sigma_n^{kk}}{dh_j}\right|_{h=0}}$$

Now we want to do a FT to momentum space.

define $$\chi_n(q) = \frac{[redacted]}{N} \sum_{R_i - R_j} \left.\frac{dG_n^{ii}}{dh_j}\right|_{h=0} e^{i\vec{q}\cdot(\vec{R}_i - \vec{R}_j)}$$

$$\Rightarrow [redacted]\, \frac{dG_n^{ii}}{dh_j} = \sum_q e^{-i\vec{q}\cdot(\vec{R}_i - \vec{R}_j)} \chi_n(q)$$

$$\chi_n^0(q) = -\frac{[redacted]}{N} \sum_{R_i - R_j} G_{ij}(i\omega_n) G_{ji}(i\omega_n) e^{i\vec{q}\cdot(\vec{R}_i - \vec{R}_j)}$$

$$\Rightarrow -[redacted]\, G_{ij}(i\omega_n) G_{ji}(i\omega_n) = \sum_q e^{-i\vec{q}\cdot(\vec{R}_i - \vec{R}_j)} \chi_n^0(q)$$

Substitute into boxed equation

$$T\sum_{q} e^{-i\vec{q}\cdot(R_i-R_j)} \chi_n(q) = T\sum_{q} e^{-i\vec{q}\cdot(R_i-R_j)} \chi_n^0(q) - T\sum_{n}\sum_{q}\sum_{k} e^{-i\vec{q}\cdot(R_i-R_k)} \chi_n^0(q)$$

$$* \left.\frac{d\Sigma_n^{kk}}{dh_j}\right|_{h=0}$$

But Σ depends only on G so

$$\frac{d\Sigma_n^{kk}}{dh_j} = \sum_m \frac{d\Sigma_n^{kk}}{dG_{kk}(i\omega_m)} \frac{dG_{kk}(i\omega_m)}{dh_j}$$

derivative can be done at $h=0$ where we have no k dependence so we get

$$\sum_q e^{-iq(R_i-R_j)} \chi_n(q) = \sum_q e^{-iq\cdot(R_i-R_j)} \chi_n^0(q) - \sum_{m}\sum_{qq'}\sum_{k} e^{-iq\cdot(R_i-R_k)} \chi_n^0(q)$$

$$* \frac{d\Sigma_n}{dG_m} \frac{1}{T} e^{-i\vec{q}'\cdot(R_k-R_j)} T\chi_m(q')$$

Sum over k sets $q=q'$ and then since this holds for ~~all~~ ~~q~~ each term in the sum separately, since it holds for all i and j we get

$$\boxed{\chi_n(q) = \chi_n^0(q) - \chi_n^0(q)\sum_m \frac{d\Sigma_n}{dG_m} \chi_m(q)}$$

define the irreducible vertex function by (static)

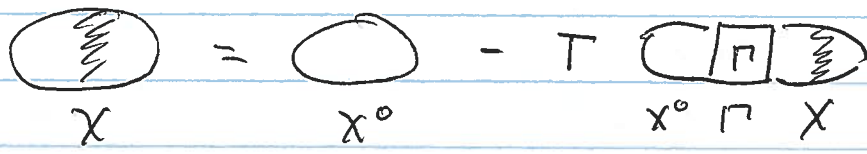
$$\Gamma_{nm} = \frac{1}{T}\frac{d\Sigma_n}{dG_m}$$

to get

$$\boxed{\chi_n(q) = \chi_n^0(q) - T\sum_m \chi_n^0(q)\Gamma_{nm}\chi_m(q)}$$

called the Bethe-Salpeter equation (Dyson eq'n for a susceptibility)

Schematically we draw pictures



The susceptibility becomes

$$\chi(q,T) = T \sum_n \chi_n(q).$$

We need to compute the vertex.

recall $\quad \Sigma_n = -\frac{1}{2G_n} + \frac{U}{2} \pm \frac{1}{2G_n}\sqrt{1 - 2(1-2W_1)UG_n + U^2G_n^2}$

This has explicit G_n dependence and implicit G_m dependence through W_1

$$\frac{d\Sigma_n}{dG_m} = \delta_{mn}\left(\frac{\partial \Sigma_n}{\partial G_n}\right)_{W_1} + \left(\frac{\partial \Sigma_n}{\partial W_1}\right)_{G_n} \frac{\partial W_1}{\partial G_m}$$

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so $\chi_n(q) = \chi_n^0(q) - \chi_n^0(q)\left(\frac{\partial \Sigma_n}{\partial G_n}\right)_{W_1}\chi_n(q) - \chi_n^0(q)\sum_m\left(\frac{\partial \Sigma_n}{\partial W_1}\right)_{G_n}\frac{\partial W_1}{\partial G_m}\chi_m(q)$

define $\quad \gamma(q) = \sum_m \chi_m(q)\frac{\partial W_1}{\partial G_m} \quad$ then

$$\chi_n(q) = \frac{\chi_n^0(q)\left[1 - \left(\frac{\partial \Sigma_n}{\partial W_1}\right)_{G_n}\gamma(q)\right]}{\left[1 + \chi_n^0(q)\left(\frac{\partial \Sigma_n}{\partial G_n}\right)_{W_1}\right]}$$

multiply both sides by $\frac{\partial \omega_1}{\partial G_n}$ and sum over n

$$\gamma(q) = \sum_n \frac{\chi^0_n(q) \frac{\partial \omega_1}{\partial G_n}\left[1 - \left(\frac{\partial \Sigma_n}{\partial \omega_1}\right)_{G_n} \gamma(q)\right]}{\left[1 + \chi^0_n(q)\left(\frac{\partial \Sigma_n}{\partial G_n}\right)_{\omega_1}\right]}$$

$$\gamma(q) = \sum_n \frac{\chi^0_n(q) \frac{\partial \omega_1}{\partial G_n}}{1 + \chi^0_n(q)\left(\frac{\partial \Sigma_n}{\partial G_n}\right)_{\omega_1}} \Bigg/ \left[1 + \sum_{n'} \frac{\chi^0_{n'}(q) \frac{\partial \omega_1}{\partial G_{n'}}\left(\frac{\partial \Sigma_{n'}}{\partial \omega_1}\right)_{G_{n'}}}{1 + \chi^0_{n'}(q)\left(\frac{\partial \Sigma_{n'}}{\partial G_{n'}}\right)_{\omega_1}}\right]$$

Define $\quad z_n = i\omega_n + \mu - \lambda_n = G_0^{-1}(i\omega_n) = G_n^{-1} + \Sigma_n$

ω_1 is an explicit function of z_n so

$$\frac{\partial \omega_1}{\partial G_n} = \sum_m \frac{\partial \omega_1}{\partial z_m}\frac{\partial z_m}{\partial G_n} \qquad z_m = G_m^{-1} + \Sigma_m$$

$$= \sum_m \frac{\partial \omega_1}{\partial z_m}\left[-\frac{\delta_{mn}}{G_n^2} + \left(\frac{\partial \Sigma_n}{\partial G_n}\right)_{\omega_1}\delta_{mn} + \left(\frac{\partial \Sigma_m}{\partial \omega_1}\right)_{G_m}\frac{\partial \omega_1}{\partial G_n}\right]$$

or $$\frac{\partial \omega_1}{\partial G_n} = \frac{\frac{\partial \omega_1}{\partial z_n}\left(-\frac{1}{G_n^2} + \left(\frac{\partial \Sigma_n}{\partial G_n}\right)_{\omega_1}\right)}{1 - \sum_m \frac{\partial \omega_1}{\partial z_m}\left(\frac{\partial \Sigma_m}{\partial \omega_1}\right)_{G_m}}$$

plug into $\gamma(q)$ expression

$$\gamma(q) = \frac{\displaystyle\sum_n \frac{\chi^0_n(q)\,\frac{\partial \omega_1}{\partial z_n}\left(-\frac{1}{G_n^2} + \left(\frac{\partial \Sigma_n}{\partial G_n}\right)_{\omega_1}\right)}{\left(1 - \sum_m \frac{\partial \omega_1}{\partial z_m}\left(\frac{\partial \Sigma_m}{\partial \omega_1}\right)_{G_m}\right)\left(1 + \chi^0_n(q)\left(\frac{\partial \Sigma_n}{\partial G_n}\right)_{\omega_1}\right)}}{\displaystyle 1 + \sum_{n'} \frac{\chi^0_{n'}(q)\,\frac{\partial \omega_1}{\partial z_{n'}}\left(-\frac{1}{G_{n'}^2} + \left(\frac{\partial \Sigma_{n'}}{\partial G_{n'}}\right)_{\omega_1}\right)\left(\frac{\partial \Sigma_{n'}}{\partial \omega_1}\right)_{G_{n'}}}{\left(1 - \sum_{m'} \frac{\partial \omega_1}{\partial z_{m'}}\left(\frac{\partial \Sigma_{m'}}{\partial \omega_1}\right)_{G_{m'}}\right)\left(1 + \chi^0_{n'}(q)\left(\frac{\partial \Sigma_{n'}}{\partial G_{n'}}\right)_{\omega_1}\right)}}$$

multiply num & den by $\left(1 - \sum_m \frac{\partial \omega_1}{\partial z_m}\left(\frac{\partial \Sigma_m}{\partial \omega_1}\right)_{G_m}\right)$

$$\gamma(q) = \frac{\displaystyle\sum_n \frac{\chi^0_n(q)\,\frac{\partial \omega_1}{\partial z_n}\left(-\frac{1}{G_n^2} + \left(\frac{\partial \Sigma_n}{\partial G_n}\right)_{\omega_1}\right)}{1 + \chi^0_n(q)\left(\frac{\partial \Sigma_n}{\partial G_n}\right)_{\omega_1}}}{\displaystyle 1 - \sum_{n'} \frac{\partial \omega_1}{\partial z_{n'}}\left(\frac{\partial \Sigma_{n'}}{\partial \omega_1}\right)_{G_{n'}} + \sum_{n'} \frac{\chi^0_{n'}(q)\,\frac{\partial \omega_1}{\partial z_{n'}}\left(-\frac{1}{G_{n'}^2} + \left(\frac{\partial \Sigma_{n'}}{\partial G_{n'}}\right)_{\omega_1}\right)\left(\frac{\partial \Sigma_{n'}}{\partial \omega_1}\right)_{G_{n'}}}{1 + \chi^0_{n'}(q)\left(\frac{\partial \Sigma_{n'}}{\partial G_{n'}}\right)_{\omega_1}}}$$

$$= \frac{\displaystyle\sum_n \frac{\chi^0_n(q)\,\frac{\partial \omega_1}{\partial z_n}\left(-\frac{1}{G_n^2} + \left(\frac{\partial \Sigma_n}{\partial G_n}\right)_{\omega_1}\right)}{1 + \chi^0_n(q)\left(\frac{\partial \Sigma_n}{\partial G_n}\right)_{\omega_1}}}{\displaystyle 1 + \sum_{n'} \frac{\partial \omega_1}{\partial z_{n'}}\left(\frac{\partial \Sigma_{n'}}{\partial \omega_1}\right)_{G_{n'}} \frac{\left(-1 \cancel{- \chi^0_{n'}(q)\left(\frac{\partial \Sigma_{n'}}{\partial G_{n'}}\right)_{\omega_1}} - \frac{\chi^0_{n'}}{G_{n'}^2} \cancel{+ \chi^0_{n'}(q)\left(\frac{\partial \Sigma_{n'}}{\partial G_{n'}}\right)_{\omega_1}}\right)}{1 + \chi^0_{n'}(q)\left(\frac{\partial \Sigma_{n'}}{\partial G_{n'}}\right)_{\omega_1}}}$$

divide all terms by $\chi^0_n(q)$ to get

$$\gamma(q) = \frac{\displaystyle\sum_n \frac{\frac{\partial \omega_1}{\partial z_n}\left(-\frac{1}{G_n^2} + \left(\frac{\partial \Sigma_n}{\partial G_n}\right)_{\omega_1}\right)}{\chi^0_n(q)^{-1} + \left(\frac{\partial \Sigma_n}{\partial G_n}\right)_{\omega_1}}}{\displaystyle 1 + \sum_{n'} \frac{\partial \omega_1}{\partial z_{n'}}\left(\frac{\partial \Sigma_{n'}}{\partial \omega_1}\right)_{G_{n'}} \frac{\left(-\chi^0_{n'}(q)^{-1} - \frac{1}{G_{n'}^2}\right)}{\chi^0_{n'}(q)^{-1} + \left(\frac{\partial \Sigma_{n'}}{\partial G_{n'}}\right)_{\omega_1}}}$$

Define $\eta_n(q) = G_n\left[-\frac{1}{G_n^2} - \chi^0_n(q)^{-1}\right]$

$$\chi^0_n(q)^{-1} = -\frac{1}{G_n^2} - \frac{\eta_n(q)}{G_n}$$

Subst in and multiply num & denom by G_n^2 to get

$$\boxed{\gamma(q) = \frac{\displaystyle\sum_n \frac{\frac{d\omega_1}{dZ_n}\left[1 - G_n^2\left(\frac{\partial \Sigma_n}{\partial G_n}\right)_{\omega_1}\right]}{1 - G_n^2\left(\frac{\partial \Sigma_n}{\partial G_n}\right)_{\omega_1} + G_n\eta_n(q)}}{1 - \displaystyle\sum_{n'} \frac{G_{n'}\eta_{n'}(q)\left(\frac{\partial \Sigma_{n'}}{\partial \omega_1}\right)_{G_{n'}}\frac{\partial \omega_1}{\partial Z_{n'}}}{1 - G_{n'}^2\left(\frac{\partial \Sigma_{n'}}{\partial G_{n'}}\right)_{\omega_1} + G_{n'}\eta_{n'}(q)}}}$$

And we recall that

$$\chi(q) = T\sum_n \chi_n(q) = T\sum_n \frac{\chi^0_n(q)\left[1 - \left(\frac{\partial \Sigma_n}{\partial \omega_1}\right)_{G_n}\gamma(q)\right]}{1 + \chi^0_n(q)\left(\frac{\partial \Sigma_n}{\partial G_n}\right)_{\omega_1}}$$

$$\boxed{\chi(q) = -T\sum_n \frac{\left[1 - \left(\frac{\partial \Sigma_n}{\partial \omega_1}\right)_{G_n}\gamma(q)\right] G_n^2}{1 - G_n^2\left(\frac{\partial \Sigma_n}{\partial G_n}\right)_{\omega_1} + G_n\eta_n(q)}}$$