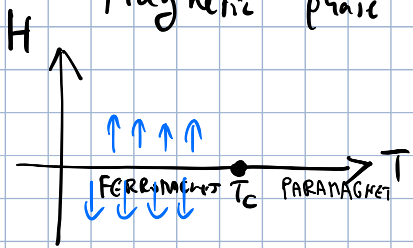
FROM MICROSCOPIC MODELS TO LANDAU THEORY

PHENOMENOLOGICAL LANDAU THEORY OF PHASE TRANSITIONS - REVIEW

Magnetic phase transitions.

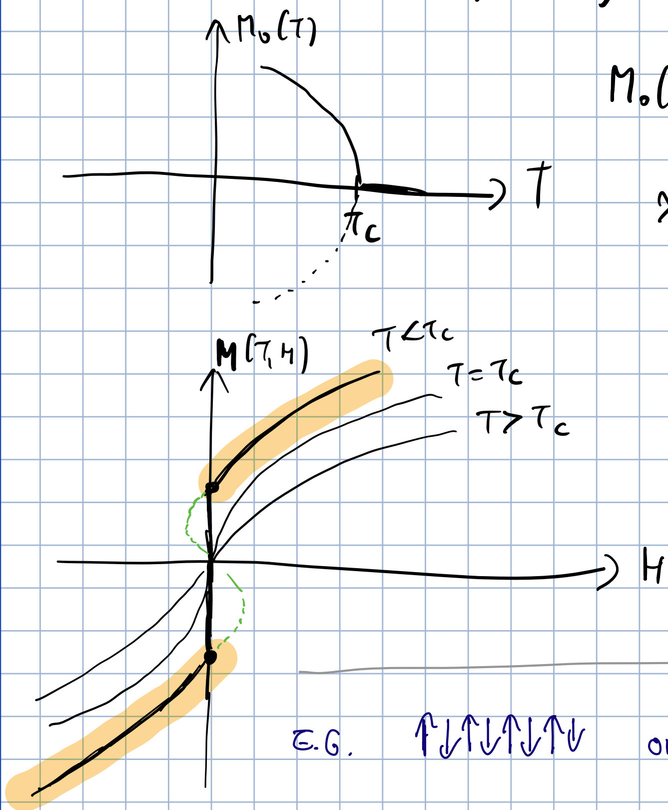


$M(T,H)$ $\qquad$ $T<T_c$ $\quad M(T,H) \xrightarrow{H \to 0^+} M_0(T)$

$\qquad\qquad\qquad\qquad\qquad\quad M(T,H) \xrightarrow{H \to 0^-} -M_0(T)$

(Our interest: $H=0$)

(Uniaxial ferromagnet)



$$M_0(T) \overset{T \to T_c^-}{\sim} (T_c - T)^{\beta} \qquad \beta \simeq 0.32$$

$$\chi = \left(\frac{\partial M}{\partial H}\right)_T \qquad \chi \sim |T - T_c|^{-\gamma}$$

$$\gamma \approx 1.24$$

(FERROMAGNETIC TRANSITION) ↑↑↑↑↑

E.G. ↑↓↑↓↑↓↑↓ OR ↑↑↓↓↑↑↓↓ → ANTIFERROMAGNETISM

Phenomenological Landau theory → APPLICABLE NOT ONLY TO MAGNETS!

$L(T, \tilde{M}, H \ldots)$

2) Description of a 2nd order phase transition

Equilibrium M is such that $L(T, \tilde{M}, H \ldots)$ has a global minimum for $\tilde{M} = M$. $\quad L(T, M(T,H) \ldots) = G(T,H)$

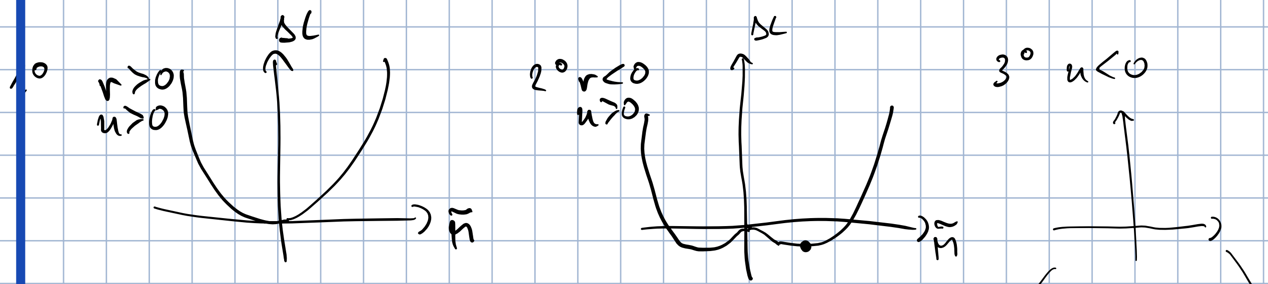
L inherits symmetries of the system.

L is analytical. (by assumption)

Focus on $H = 0$, M SMALL IN THE VICINITY OF PHASE TRANSITION.

$$L(T, \tilde{M}, 0 \ldots) = L(T,0,0) + \frac{1}{2} r(T) \tilde{M}^2 + \frac{1}{4!} u(T) \tilde{M}^4 + \ldots$$

$$\Delta L(T, \tilde{M}, 0) = L(T, \tilde{M}, 0) - L(T,0,0) = \frac{1}{2} r(T) \tilde{M}^2 + \frac{1}{4!} u(T) \tilde{M}^4 + \ldots$$



Not relevant for the present physical situation.

$$r(T) = \underbrace{r(T_c)}_{=0} + r'(T_c)(T - T_c) + \ldots$$

$$u(T) = u(T_c) + \ldots = u$$

$$\tau := \frac{T - T_c}{T_c}$$

$$\Delta L = \frac{1}{2} \overset{\text{const}}{a} \tau \tilde{M}^2 + \frac{u}{4!} \tilde{M}^4$$

$$\frac{\partial \Delta L}{\partial \tilde{M}} = 0 \qquad 0 = a\tau \tilde{M} + \frac{u}{3!} \tilde{M}^3 \qquad \tilde{M}\left(a\tau + \frac{u}{3!} \tilde{M}^2\right) = 0.$$

$\tau > 0 \qquad \tilde{M} = M = 0$

$\tau < 0 \qquad \tilde{M} = M = \pm\sqrt{\frac{6a\tau}{-u}} \qquad M \sim |\tau|^{\beta} \qquad \beta = \frac{1}{2}.$

- universal
- $\beta = 0.32$

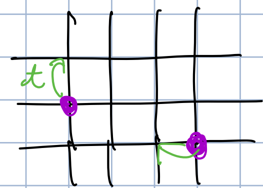
In what follows $\tilde{M} \Leftrightarrow \phi$

QUESTION: Can one make a connection between Landau theory and microscopic physics?

↳ What is $\mathcal{L}$ from the stat. physics point of view?

Imagine we have a specific H to begin with.

E.g. $$H = \underbrace{\sum_{\bar{\ell}\bar{\ell}'\sigma} t_{\bar{\ell}-\bar{\ell}'}\, a^{+}_{\bar{\ell}\sigma} a_{\bar{\ell}'\sigma}}_{\xrightarrow{\text{F.T.}} \left\{\sum_{\bar{k}\sigma} \epsilon_{\bar{k}}\, a^{+}_{\bar{k}\sigma} a_{\bar{k}\sigma}\right\}} + U \sum_{\bar{\ell}} \hat{n}_{\bar{\ell}\uparrow} \hat{n}_{\bar{\ell}\downarrow}$$ (HUBBARD MODEL)



$\mathcal{H} = H - \mu \hat{N}$

$\hat{N} = \sum_{\bar{\ell}\sigma} \hat{n}_{\bar{\ell}\sigma}$

$\hat{n}_{\bar{\ell}\sigma} = a^{+}_{\bar{\ell}\sigma} a_{\bar{\ell}\sigma}$ (FERMIONS) $d \in \{2, 3\}$

$U > 0$

Electrons on a lattice, simple (here onsite) interaction.

$Z = \mathrm{Tr}\, e^{-\beta \mathcal{H}}$, $\Omega = -k_B T \ln Z$

→ Horribly complicated problem... (Many possible phase transitions...)

Not much progress possible without additional assumptions/approximations.
(numerics very useful).

For now: focus on magnetic properties: $H_U = U \sum_{\bar{\ell}} \hat{n}_{\bar{\ell}\uparrow}\hat{n}_{\bar{\ell}\downarrow} = \frac{U}{4} \sum_{\bar{\ell}} \Big[\underbrace{(\hat{n}_{\bar{\ell}\uparrow} + \hat{n}_{\bar{\ell}\downarrow})^2}_{\text{charge}} - \underbrace{(\hat{n}_{\bar{\ell}\uparrow} - \hat{n}_{\bar{\ell}\downarrow})^2}_{\text{magnetization}} \Big]$

↓

drop the charge term. ↳ This takes us away from "real solution" of the model.

Recall the path integral for Z:

$$\boxed{Z = \int_{\substack{\xi(\beta) = \zeta \xi(0) \\ \xi^*(\beta) = \zeta \xi^*(0)}} \mathcal{D}[\xi^*, \xi]\, e^{-S[\xi^*, \xi]} \qquad S[\xi^*, \xi] = \int_0^\beta d\tau \Big[\sum_\alpha \xi^*_\alpha(\tau) \partial_\tau \xi_\alpha(\tau) + \mathcal{H}\big(\xi^*_\alpha(\tau^+), \xi_\alpha(\tau)\big) \Big]}$$

(FERMIONS $\zeta = -1$)

the "hard" term

$$Z = \int \mathcal{D}[\xi^* \xi]\, e^{-\int_0^\beta d\tau \Big[\sum_{\bar{\ell}\sigma} \xi^*_{\bar{\ell}\sigma}(\tau) \partial_\tau \xi_{\bar{\ell}\sigma}(\tau) + \sum_{\bar{\ell}\bar{\ell}'\sigma} (t_{\bar{\ell}-\bar{\ell}'} - \mu \delta_{\bar{\ell}\bar{\ell}'}) \xi^*_{\bar{\ell}\sigma}(\tau) \xi_{\bar{\ell}'\sigma}(\tau) - \frac{U}{4} \sum_{\bar{\ell}} (\tilde{n}_{\bar{\ell}\uparrow}(\tau) - \tilde{n}_{\bar{\ell}\downarrow}(\tau))^2 \Big]}$$

$\tilde{n}_{\bar{\ell}\sigma}(\tau) = \xi^*_{\bar{\ell}\sigma}(\tau)\, \xi_{\bar{\ell}\sigma}(\tau)$

{recall: $\int d\tau \longleftrightarrow \sum_{\bar{\ell}}$ }

AIM: MAKE CONNECTION TO LANDAU THEORY.

④

Integral identity: $e^{\frac{b^2}{2a}} = \sqrt{\frac{a}{2\pi}} \int_{-\infty}^{\infty} d\phi\, e^{-\frac{a}{2}\phi^2 + b\phi}$ $(a>0)$ $(*)$

(HUBBARD–STRATONOVICH TRANSFORMATION)

Associate $\begin{cases} a \leftrightarrow \frac{1}{2}U \\ b^2 \leftrightarrow \left(\frac{1}{2}U\right)^2 (\tilde{n}_{\bar{\ell}\uparrow} - \tilde{n}_{\bar{\ell}\downarrow})^2 \end{cases}$

Apply $(*)$ for each $(\bar{\ell}, \tau)$

$\to \phi \longrightarrow \phi_{\bar{\ell}}(\tau)$

$$e^{\int_0^\beta d\tau \frac{U}{4} \sum_{\bar{\ell}} (\tilde{n}_{\bar{\ell}\uparrow}(\tau) - \tilde{n}_{\bar{\ell}\downarrow}(\tau))^2} = \underbrace{\int \prod_{\bar{\ell}\tau} \left(\sqrt{\frac{U}{4\pi}} d\phi_{\bar{\ell}}(\tau) \right)}_{:= \int \mathcal{D}\phi_{\bar{\ell}}(\tau)} e^{-\int_0^\beta d\tau \sum_{\bar{\ell}} \left[\frac{U}{4}\phi_{\bar{\ell}}^2(\tau) + \frac{U}{2}(\tilde{n}_{\bar{\ell}\uparrow}(\tau) - \tilde{n}_{\bar{\ell}\downarrow}(\tau))\phi_{\bar{\ell}}(\tau) \right]}$$

$$Z = \int \mathcal{D}[\xi^* \xi] \int \mathcal{D}\phi_{\bar{\ell}}(\tau)\, e^{-\int_0^\beta d\tau \left[\sum_{\bar{\ell}\sigma} \xi^*_{\bar{\ell}\sigma}(\tau)\partial_\tau \xi_{\bar{\ell}\sigma}(\tau) + \sum_{\bar{\ell}\bar{\ell}'\sigma} (t_{\bar{\ell}-\bar{\ell}'} - \mu\delta_{\bar{\ell}\bar{\ell}'}) \xi^*_{\bar{\ell}\sigma}(\tau)\xi_{\bar{\ell}'\sigma}(\tau) + \sum_{\bar{\ell}} \frac{U}{4}\phi_{\bar{\ell}}^2(\tau) + (\tilde{n}_{\bar{\ell}\uparrow}(\tau) - \tilde{n}_{\bar{\ell}\downarrow}(\tau)) \frac{U}{2}\phi_{\bar{\ell}}(\tau) \right]}$$

linear coupling between ϕ and magnetization

The argument of the exponent is a quadratic form in (ξ^*, ξ) → can do the $\mathcal{D}[\xi^* \xi]$ integration

$$Z = \int \mathcal{D}\phi_{\bar{\ell}}(\tau) \int \mathcal{D}[\xi^* \xi]\, e^{-S[\xi^*, \xi, \phi]}$$

$$\left(\tilde{n}_{\bar{\ell}\uparrow}(\tau) - \tilde{n}_{\bar{\ell}\downarrow}(\tau)\right) = \xi^*_{\bar{\ell}\uparrow}(\tau)\xi_{\bar{\ell}\uparrow}(\tau) - \xi^*_{\bar{\ell}\downarrow}(\tau)\xi_{\bar{\ell}\downarrow}(\tau) = \sum_\sigma \xi^*_{\bar{\ell}\sigma}(\tau)\xi_{\bar{\ell}\sigma}(\tau)\,\sigma$$

$$S[\xi^*, \xi, \phi] = \int_0^\beta d\tau \int_0^\beta d\tau' \sum_{\bar{\ell}\bar{\ell}'} \sum_{\sigma\sigma'} \Big\{ \xi^*_{\bar{\ell}'\sigma'}(\tau')\, \delta(\tau-\tau') \Big[\delta_{\bar{\ell}\bar{\ell}'}\delta_{\sigma\sigma'}(\partial_\tau - \mu) + \delta_{\sigma\sigma'} t_{\bar{\ell}-\bar{\ell}'} + \frac{U}{2}\delta_{\bar{\ell}\bar{\ell}'}\delta_{\sigma\sigma'}\,\sigma\,\phi_{\bar{\ell}}(\tau) \Big] \xi_{\bar{\ell}\sigma}(\tau) \Big\} + \int_0^\beta d\tau \sum_{\bar{\ell}} \frac{U}{4}\phi_{\bar{\ell}}^2(\tau)$$

$$\int \mathcal{D}[\xi^* \xi]\, e^{-\xi^* \mathbb{A} \xi} = \det \mathbb{A} = e^{\ln\det \mathbb{A}} = e^{\mathrm{Tr}\ln \mathbb{A}}$$

$$Z = \int \mathcal{D}\phi_{\bar{\ell}}(\tau)\, e^{-A[\phi]} \qquad A[\phi] = \int_0^\beta d\tau \sum_{\bar{\ell}} \frac{U}{4}\phi_{\bar{\ell}}^2(\tau) - \mathrm{Tr}\ln[\mathbb{M}]$$

$$\xi_{\bar l\sigma}(\tau) = \sum_{\bar k\,\omega_n} \xi_{\bar k\omega_n\sigma}\, e^{i(\bar k\bar l-\omega_n\tau)}\frac{1}{\sqrt{\beta N_0}}$$

$$\xi^*_{\bar l\sigma}(\tau) = \sum_{\bar k\,\omega_n} \xi^*_{\bar k\omega_n\sigma}\, e^{-i(\bar k\bar l-\omega_n\tau)}\frac{1}{\sqrt{\beta N_0}}$$

$$\phi_{\bar l}(\tau) = \sum_{q\,\omega_m} \phi_{\bar q\omega_m\sigma}\, e^{i(\bar q\bar l-\omega_m\tau)}\frac{1}{\sqrt{\beta N_0}}$$

- τ integration $\rightarrow$ $\delta_{\omega_n-\omega_n'}$ or $\delta_{\omega_n'-\omega_n-\omega_m}$ $(\times\beta)$
- (second term) $\sum_{\bar l\bar l'} t_{\bar l-\bar l'}\, e^{-i\bar k'\bar l'} e^{i\bar k\bar l} = \underbrace{\sum_{\bar x} t_{\bar x}\, e^{i\bar k'\bar x}}_{=\varepsilon_{\bar k'}} e^{i(\bar k-\bar k')\bar l}$

$$S[\xi^*,\xi,\phi] = \int_0^\beta d\tau \int_0^\beta d\tau' \sum_{\bar l\bar l'}\sum_{\sigma\sigma'}\Big\{\xi^*_{\bar l'\sigma'}(\tau')\,\delta(\tau-\tau')\Big[\delta_{\bar l\bar l'}\,\delta_{\sigma\sigma'}(\partial_\tau-\mu)+\delta_{\sigma\sigma'}\,t_{\bar l-\bar l'}+$$
$$+\frac{u}{2}\delta_{\bar l\bar l'}\,\delta_{\sigma\sigma'}\,\sigma\,\phi_{\bar l}(\tau)\Big]\xi_{\bar l\sigma}(\tau)\Big\} + \int_0^\beta d\tau \sum_{\bar l}\frac{u}{4}\phi^2_{\bar l}(\tau)$$

$$S[\xi^*,\xi,\phi] = \sum_{\bar k\bar k'}\sum_{\omega_n\omega_n'}\sum_{\sigma\sigma'}\Big\{\xi^*_{\bar k'\omega_n'\sigma'}\underbrace{\Big[\overbrace{\delta_{\sigma\sigma'}\big[-i\omega_n+\xi_{\bar k}\big]\delta_{\omega_n,\omega_n'}\,\delta_{\bar k\bar k'}}^{-G_0^{-1}}+\overbrace{\frac{1}{\sqrt{\beta N}}\,\sigma\,\frac{u}{2}\,\phi(\bar k-\bar k',\,i\omega_n-i\omega_n')}^{V}\Big]}_{\mathbb{M}}\xi_{\bar k\omega_n\sigma}\Big\}+$$
$$+\sum_{\bar q,\omega_m}\frac{u}{4}\,\phi_{\bar q,\omega_m}\,\phi_{-\bar q,-\omega_m}$$

$$\left\{\int \mathcal{D}[\xi^*\xi]\, e^{-\xi^*\mathbb{A}\xi} = \det\mathbb{A} = e^{\ln\det\mathbb{A}} = e^{\mathrm{Tr}\ln\mathbb{A}}\right\}$$

$$Z = \int \mathcal{D}\phi\, e^{-A[\phi]}$$

$$A[\phi] = \int_0^\beta d\tau \sum_{\bar l}\frac{u}{4}\phi^2_{\bar l}(\tau) - \mathrm{Tr}\ln\big[\mathbb{M}\big]$$

Relation to Landau theory:

→ EXPAND $\mathcal{A}[\phi]$ in ϕ

→ TREAT $\int \mathcal{D}\phi \, e^{-\mathcal{A}[\phi]}$ WITH SADDLE-POINT APPROXIMATION

$$\mathcal{G}[T, H=0] = -T \ln Z = -T \ln \int \mathcal{D}\phi \, e^{-\mathcal{A}[\phi]} \approx$$

$$\approx -T \ln e^{-\mathcal{A}[\phi_0]} = T\mathcal{A}[\phi_0]$$

$$\mathcal{A}[\phi] \Leftrightarrow L[\phi] \quad !!!$$

Next class:

- EVALUATE THE ϕ EXPANSION
- EVALUATE THE q, ω EXPANSION
- EXAMPLES/OVERVIEW.

$$\mathrm{Tr} \ln \mathbb{M} = \mathrm{Tr} \ln\left[-G_0^{-1} + V\right] = \mathrm{Tr} \ln\left[-G_0^{-1}\left(1 - G_0 V\right)\right] =$$

$$= \mathrm{Tr} \ln\left[-G_0^{-1}\right] + \mathrm{Tr} \ln\left(1 - G_0 V\right) =$$

$$= \mathrm{Tr} \ln\left[-G_0^{-1}\right] - \sum_{n=1}^{\infty} \frac{1}{n} \mathrm{Tr}\left(G_0 V\right)^n$$

$$\xi_{l\sigma}(\tau) = \sum_{\bar{k}\,\omega_n} \xi_{\bar{k}\omega_n\sigma} e^{i(\bar{k}\bar{l}-\omega_n\tau)} \frac{1}{\beta N_0}$$

$$\xi^*_{l\sigma}(\tau) = \sum_{\bar{k}\,\omega_n} \xi^*_{\bar{k}\omega_n\sigma} e^{-i(\bar{k}\bar{l}-\omega_n\tau)} \frac{1}{\beta N_0}$$

$$\phi_l(\tau) = \sum_{\bar{q}\,\omega_m} \phi_{\bar{q}\omega_m\sigma} e^{i(\bar{q}\bar{l}-\omega_m\tau)} \frac{1}{\beta N_0}$$

$$\int_0^\beta d\tau \int_0^\beta d\tau' \sum_{ll'} \sum_{\sigma\sigma'} \left\{ \dots \right\} = \int_0^\beta d\tau \sum_{\bar{l}\bar{l}'\sigma} \left\{ \sum_{\bar{k}'\omega_n'} \xi^*_{\bar{k}'\omega_n'} e^{-i(\bar{k}'\bar{l}'-\omega_n'\tau)} \Big[\delta_{ll'}(-i\omega_n-\mu) \right.$$

$$\left. + t_{\bar{l}-\bar{l}'} + \delta_{ll'}\sigma \sum_{\bar{q}\omega_m} \phi_{\bar{q}\omega_m} e^{i(\bar{q}\bar{l}-\omega_m\tau)} \Big] \sum_{\bar{k}\omega_n} \xi_{\bar{k}\omega_n} e^{i(\bar{k}\bar{l}-\omega_n\tau)} \right\}$$

- τ integration $\rightarrow$ $\delta_{\omega_n-\omega_n'}$ or $\delta_{\omega_n'-\omega_n-\omega_m}$ $(\times\beta)$
- (second term) $\sum_{\bar{l}\bar{l}'} t_{\bar{l}-\bar{l}'} e^{-i\bar{k}'\bar{l}'} e^{i\bar{k}\bar{l}} = \underbrace{\sum_{\bar{x}} t_{\bar{x}} e^{i\bar{k}'\bar{x}}}_{=\epsilon_{\bar{k}'}} e^{i(\bar{k}-\bar{k}')\bar{l}}$

$$= \sum_{\bar{k}\bar{k}'} \sum_{\omega_n\omega_n'} \sum_{\sigma} \xi^*_{\bar{k}'\omega_n'\sigma'} \left\{ \delta_{\sigma\sigma'} \Big[\delta_{\omega_n\omega_n'} \delta_{\bar{k}\bar{k}'} (-i\omega_n + \epsilon_{\bar{k}} - \mu) + \right.$$

$$\left. + \frac{1}{\beta N_0} \sigma \sum_{\bar{q}\omega_m} \phi_{\bar{q}\omega_m} \delta_{\bar{q}+\bar{k}-\bar{k}'} \delta_{\omega_m+\omega_n-\omega_n'} \Big] \right\} \xi_{\bar{k}\omega_n\sigma}$$

$$\left\{ \dots \right\} = \mathbb{M}.$$

We need $\mathrm{Tr}\ln\mathbb{M}$.

$$\delta_{\sigma\sigma'}\delta_{\omega\omega'}(-i\omega_n + \epsilon_k - \mu) \longrightarrow -G_0^{-1}$$

SECOND TERM IN $\mathbb{M} \rightarrow V$

$$\mathrm{Tr}\ln\mathbb{M} = \mathrm{Tr}\ln\left[-G_0^{-1} + V\right] = \mathrm{Tr}\ln\left[-G_0^{-1}(1 - G_0 V)\right] =$$

$$= \mathrm{Tr}\ln\left[-G_0^{-1}\right] + \mathrm{Tr}\ln\left[1-G_0V\right] =$$

$$= \mathrm{Tr}\left[-G_0^{-1}\right] - \sum_{n=1}^{\infty}\frac{1}{n}\mathrm{Tr}\left(G_0V\right)^n$$

- $\mathrm{Tr}\left(G_0V\right) = \frac{1}{\beta N_0}\sum_{\omega_n \bar{k}\sigma} G_0(i\omega_n,\bar{k})\,\sigma\,\phi_{0,0} = 0$

- $\frac{1}{2}\mathrm{Tr}\, G_0VG_0V = \frac{1}{2}\sum_{\omega_n\bar{k}\sigma}\sum_{\omega_n'\bar{k}'\sigma'} G_0(i\omega_n,\bar{k})(V)_{(i\omega_n,\bar{k},\sigma),(i\omega_n',\bar{k}',\sigma')} \times$

$$\times\, G_0(i\omega_n',\bar{k}')(V)_{(i\omega_n'\bar{k}'\sigma')(i\omega_n,\bar{k},\sigma)} =$$

$$= \frac{1}{2}\sum_{\dots}\frac{1}{(\beta N_0)^2}\cdot \overset{\sigma\text{ summation}}{2}\, G_0(i\omega_n,\bar{k})\,\phi_{i\omega_n-i\omega_n',\bar{k}-\bar{k}'}\,G_0(i\omega_n',\bar{k}')\cdot$$

$$\cdot\,\phi_{i\omega_n'-i\omega_n,\bar{k}'-\bar{k}} =$$

$$= \frac{1}{(\beta N_0)^2}\sum_{\bar{q},i\omega_m}\left(\sum_{\bar{k},i\omega_n} G_0(i\omega_n,\bar{k})\,G_0(i\omega_n+i\omega_m,\bar{k}+\bar{q})\right)\cdot$$

$$\cdot\,\phi_{i\omega_m,\bar{q}}\,\phi_{-i\omega_m,\bar{q}}$$

$(\quad) \longrightarrow$ POLARIZATION BUBBLE DIAGRAM

Up to 2nd order in V (ϕ)

$$A[\phi] = \left[\int_0^\beta d\tau \sum_l \phi_l^2(\tau)\frac{1}{U} - \right.$$  $$\left.\right]$$

FOURIER TRANSFORM $\int_0^\beta d\tau \sum_l \phi_l^2(\tau)\frac{1}{U} = \sum_{\bar{q}\,\omega_m}\phi_{\bar{q}\,\omega_m}\phi_{-\bar{q},-\omega_m}\frac{1}{U}$

$$A[\phi] = \sum_{\bar{q}\,\omega_m} \phi_{\bar{q}\,\omega_m} \Big(\frac{1}{U} -$$  $$\Big) \phi_{-\bar{q},-\omega_m} + \dots$$

$$\mathcal{Z} = \int \mathcal{D}\phi \; e^{-A[\phi]}$$

Inclusion of H.O.T in $\mathrm{Tr}\ln(G_0 V)$ generates an expansion of $A[\phi]$ in powers of ϕ $\rightarrow$ LANDAU EXPANSION !