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"Magnetic instabilities in the 2D Hubbard model at low doping"

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Magnetic instabilities in the 2D Hubbard model at low doping

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Contents

- Hubbard model

$$H = -t \sum_{\langle i,j \rangle} (c_i^+ c_j + c_j^+ c_i) + U \sum_i n_{i\uparrow} n_{i\downarrow}$$

- $T=0$, single dimensionless ratio $8t/U$

- experiment $8t/U = O(1)$

- theory $\nearrow$ $t \ll U$ ($t-J$, no double occupancy)
  $\searrow$ $t \gg U$ (RPA)

- Is there a smooth crossover between the two limits?

- half filling - AFM ground state $\Rightarrow$
$\Rightarrow$ a gap in the electronic spectrum $\Rightarrow$ insulator

Away from h.f.?

Immediate incommensurability (mean field)
(domain walls, Schulz)
(spiral phase, Shraiman & Siggia)
* (superconductivity due to "spin bags", Schrieffer, Wen, Zhang)

Our results

1) no immediate instability of a commensurate AFM state

2) for larger doping concentrations, spiral instability may occur, but its possibility is not governed by a large parameter

3) the transition, if occurs, is not due to softening of spin-wave excitations

4) no superconducting instability at low doping

Hubbard model at half-filling

- introduce spin density operators

$$\vec{S}(q) = \frac{1}{2} \sum a^{+}_{k+q,\alpha} \, \vec{\sigma}_{\alpha\beta} \, a_{k,\beta}$$

- antiferromagnetism : $\langle S_z(q=(\pi,\pi)) \rangle \neq 0$

- mean field
  a) decoupling of the quartic term
  b) diagonalization of the quadratic form
  c) self-consistency condition

- $$H = \sum_{k,\sigma}{}' E_k \left(c^{+}_{k,\sigma} c_{k\sigma} - d^{+}_{k,\sigma} d_{k,\sigma} \right)$$

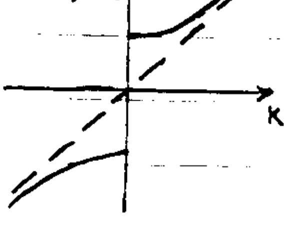
$$E_k = \sqrt{\varepsilon_k^2 + \Delta^2}, \quad \varepsilon_k = -2t(\cos k_x + \cos k_y)$$

$$\Delta = U \langle S_z \rangle, \quad \boxed{\frac{1}{U} = \sum_k{}' 1/E_k}$$

- $U \gg t$, $\Delta \simeq U/2$ $\left(\langle S_z \rangle = 1/2\right)$

- $U \ll t$, Van-Hove + nesting $\Rightarrow$ double ln singularity of $\sum_k \frac{1}{\varepsilon_k}$

$$\Delta = t \, e^{-2\pi\sqrt{t/U}}$$



c_k - conduction band
d_k - valence band

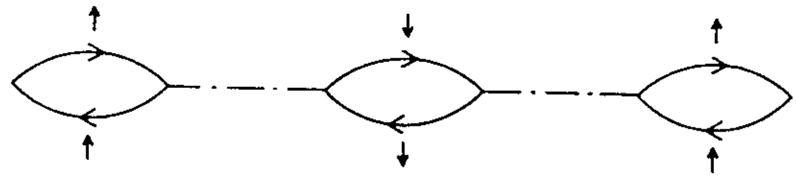
* collective excitations

$$\chi^{ij}(q,q',\omega) = \int dt\, e^{i\omega t}\left[\frac{i}{2N}\langle T\, S^i_q(t)\, S^j_{-q'}(0)\rangle\right]$$

$\langle\vec{S}\rangle \neq 0 \Rightarrow$ Goldstone modes

RPA

χ^{zz} :



Generally, $\chi^{ij}(q,q',\omega) \neq 0$ at $\begin{cases} q = q' \\ q = q' + Q, \quad Q = (\pi,\pi) \end{cases}$

$$\chi^{+-}(q,q,\omega) = \frac{\chi_0^{+-}(q,\omega)\left[1 - U\chi_0^{+-}(q+Q,\omega)\right] + U(\chi_Q^{+-}(q,\omega))^2}{\left(1 - U\chi_0^{+-}(q,\omega)\right)\left(1 - U\chi_0^{+-}(q+Q,\omega)\right) - U^2(\chi_Q^{+-}(q,\omega))^2}$$

$$\chi_0^{+-}(q,\omega) = \frac{1}{2N}\sum_k{}'\left(1 - \frac{\varepsilon_k\varepsilon_{k+q} - \Delta^2}{E_k E_{k+q}}\right)\left(\frac{1}{E_k + E_{k+q} - \omega} + \frac{1}{E_k + E_{k+q} + \omega}\right)$$

$$\chi_Q^{+-}(q,\omega) \equiv \chi_0^{+-}(q, q+Q, \omega) =$$

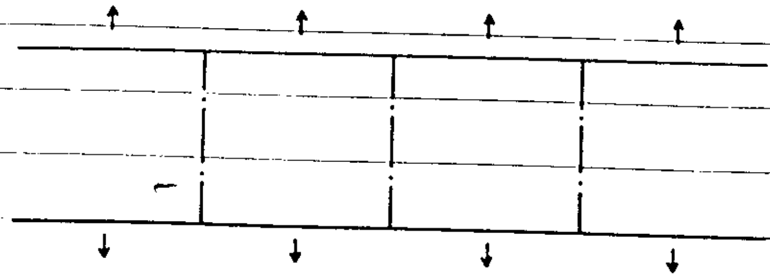
$$= \frac{1}{2N}\sum_k{}' \frac{\Delta(E_k + E_{k+q})}{E_k E_{k+q}}\left(\frac{1}{E_k + E_{k+q} - \omega} - \frac{1}{E_k + E_{k+q} + \omega}\right)$$

1a

$$\chi_Q^{+-}(q,\omega) \sim \omega$$

(6'

χ^{+-}



1b

- poles of χ^{+-} - gapless bosonic excitations

$$1 - U\chi^{+-}(q=Q, \omega=0) \equiv \text{"gap" equation } \frac{1}{U} = \sum_k{}' \frac{1}{E_k}$$

- expansion around $q, \omega = 0$

$$\omega^2 = c^2 q^2$$

$c = J\sqrt{2}$, $U \gg t$ $\left(J = \frac{4t^2}{U}, \quad \omega = 2J\sqrt{1-\gamma_q^2} \right.$
$\left. \gamma_q = \frac{1}{2}(\cos k_x + \cos k_y) \right)$

$c^2 = \left(\frac{4}{\pi}\right) t^2 \left(\frac{U}{t}\right)^{1/2}$, $U \ll t$ (differs from $c^2 \sim t^2$ of SWZ)

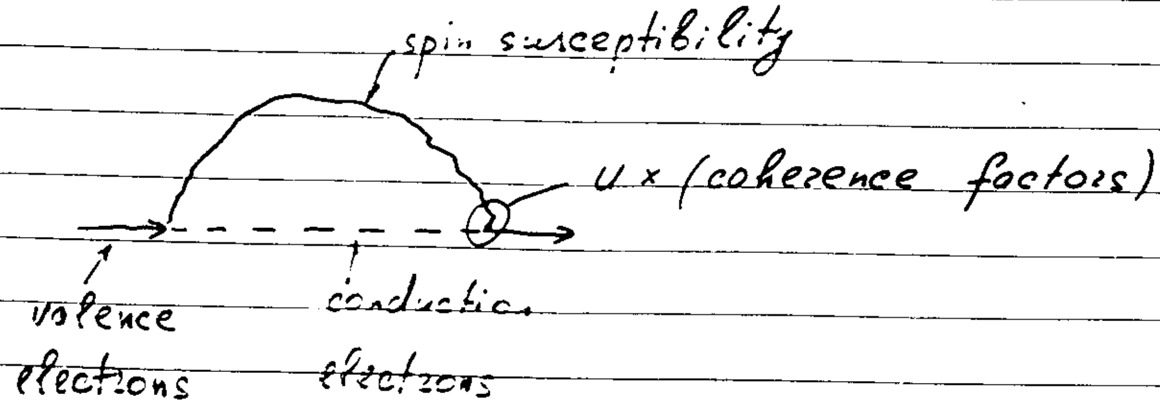
$c^2 = \rho_s / \chi_\perp$, $\chi_\perp = \chi^{xx}(q=0, \omega=0)$, $\chi^{xx}(q \approx Q, \omega) = \left. \frac{(\langle S_z \rangle)^2}{\rho_s (q-Q)^2} \right|_{\omega=0}$

- corrections to m-f $\equiv$ expansion in $1/z$ (z is the coordination number)

- comparison with SW theory (large U)

- $\langle S_z \rangle = \frac{2}{N} \sum_k{}' \langle d^+_{k\uparrow} d_{k\uparrow} \rangle - 1/2$

- quasiparticles interact with each other through collective modes



- single-particle spectrum preserves its form

- $$G = \frac{Z}{\Omega + \bar{E}_k}, \quad \bar{E}_k = \sqrt{\bar{\Delta}^2 + 4\bar{t}^2(\cos k_x + \cos k_y)^2}$$

$$Z = 1 - \frac{1}{N}\sum_k{}' \frac{1-\sqrt{1-\gamma_k^2}}{\sqrt{1-\gamma_k^2}}, \quad \bar{\Delta} = D/Z^2$$

$$\bar{t} = t\left(1 + \frac{1}{N}\sum_k{}' \frac{\gamma_k^2}{\sqrt{1-\gamma_k^2}}\right)$$

- $$\langle S_z \rangle = Z - 1/2 = \frac{1}{2}\left(1 - \frac{2}{N}\sum_k{}' \frac{1-\sqrt{1-\gamma_k^2}}{\sqrt{1-\gamma_k^2}}\right)$$

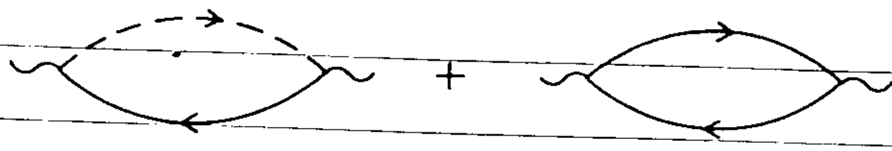
- $$\chi_\perp = \frac{1}{8J}\left(\frac{t}{\bar{t}}\right)^2 = \frac{1}{8J}\left(1 - \frac{2}{N}\sum_k{}' \frac{\gamma_k^2}{\sqrt{1-\gamma_k^2}}\right)$$

- $$e = J\sqrt{2}\left(1 + \frac{2}{N}\sum_k{}' \left(1 - \sqrt{1-\gamma_k^2}\right)\right)$$

Mean field theory at finite doping

- RPA expression for $\bar{\chi}(q, q', \omega)$ remains the same

- two types of bubbles for $\chi_0^{+-}(q,\omega)$



$$\chi_0^{+-}(q,\omega) = \frac{1}{2N} \sum_{E_{k+q}>|\mu|}{}' \left(1 - \frac{\varepsilon_k \varepsilon_{k+q} - \Delta^2}{E_k E_{k+q}}\right) \times$$

$$\left[\frac{1}{E_k + E_{k+q} - \omega} + \frac{1}{E_k + E_{k+q} + \omega}\right]$$

$$\frac{1}{2N} \sum_{\substack{E_{k+q} > |\mu| \\ E_k < |\mu|}}{}' \left(1 + \frac{\varepsilon_k \varepsilon_{k+q} - \Delta^2}{E_k E_{k+q}}\right)\left[\frac{1}{E_{k+q} - E_k - \omega} - \frac{1}{E_k - E_{k+q} - \omega}\right]$$

3a

- static susceptibility

$$(\bar{\chi}^{+-})^{-1} \sim 1 - u\,\chi_0^{+-}(q, \omega = 0) =$$

$$= \frac{u}{4N} \sum_{E_k > \mu}{}' \frac{(\varepsilon_k + \varepsilon_{k+q})^2}{E_k^3} - \frac{u}{2N} \sum_{\substack{E_{k+q} > |\mu| \\ E_k < |\mu|}}{}' \frac{(\varepsilon_k + \varepsilon_{k+q})^2}{E_k E_{k+q}} \frac{1}{E_{k+q} - E_k}$$

near $q = Q$, $(\varepsilon_k + \varepsilon_{k+q}) \sim q - Q \equiv \bar{q}$

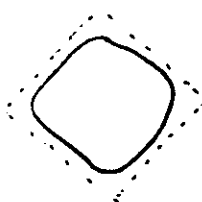
$$\boxed{\rho_s = \rho_s^{(0)} \left(1 - \Gamma^{+-} \tilde{\chi}^{+-}\right)}$$

$$\tilde{\chi}^{+-} = \frac{2}{N} \sum_{\substack{E_{k+q} > |\mu| \\ E_k < |\mu|}}{}' \frac{1}{E_{k+q} - E_k} \cdot \frac{(q_x \sin k_x + q_y \sin k_y)^2}{q^2}$$

$$\Gamma^{+-} \sim \begin{cases} t, & u \ll t \\ u, & u \gg t \end{cases}$$

- Fermi surface

$E_k = \mu \Rightarrow 2t(\cos k_x + \cos k_y) = \varepsilon_F \quad (\varepsilon_F^2 = \mu^2 - \Delta^2)$



The Fermi surface stretches along the whole reduced BZ boundary

$\nu(\varepsilon_F) \sim 1/\varepsilon_F$

$$\tilde{\chi}^{+-} \sim \left(\frac{\Delta}{t}\right)\frac{1}{\varepsilon_F} \quad (!)$$

(Singh & Tesanovic, Weng & Ting)

$\rho_s < 0$ at arbitrary small doping levels

- even incommensurate ordering does not help
(Auerbach & Larson)

χ^{zz}, $\chi^{\rho\rho}$

At half filling, $$\bar{\chi}^{zz} = \frac{\chi_e(q,\omega)}{1 - u\chi_e(q,\omega)}$$

$$\chi_e(q,\omega) = \frac{1}{2N}\sum_k{}' \left(1 - \frac{\varepsilon_k\varepsilon_{k+q}+\Delta^2}{E_k E_{k+q}}\right)\left(\frac{1}{E_k+E_{k+q}-\omega} + \frac{1}{E_k+E_{k+q}+\omega}\right)$$

$$1 - u\chi_e(Q,\omega=0) \neq 0$$

In general, $\bar{\chi}^{\rho z}(q, q+Q, \omega) \neq 0$

AFM: translation by a + rotation to π around, say, X.

$$S_z(q) \to \ominus e^{iqa} S_z(q)\ ;\ \rho(q') \to e^{iq'a}\rho(q')$$

$S_z(-q')\,\rho(q'+Q)$ — inv

$$\left(\bar{\chi}^{zz}\right)^{-1} \sim 1 - \Gamma^{zz}\,\tilde{\chi}^{zz}(q)$$

Pauli-like susceptibility

$$\Gamma^{zz} = \frac{U^2\,\chi_0^{zz}(q)}{1 - U\,\chi_0^{zz}(q)}$$

- at $q = Q$, $\Gamma^{zz} \sim \begin{cases} t \times (U/t)^{1/2}, & t \ll U \\ J, & U \gg t \end{cases}$

$$\chi^{zz}(Q) = \frac{1}{\pi^2}\left(\frac{\Delta}{t}\right)\frac{1}{\varepsilon_F}\,\underbrace{\ln\frac{4t}{\varepsilon_F}}$$

from Van-Hove singularities

- immediate instabilities in χ^{+-} and χ^{zz}
- additional log in χ^{zz} (Schulz)

Renormalization effects

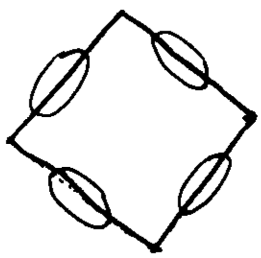
1) $\chi \sim \frac{1}{\varepsilon_F}$ is due to "open" Fermi surface

the problem is quasi 1D $\Rightarrow$ vertex renormalization

2) "open" Fermi surface is an artifact of mean-field (no symmetry reasons)

Numerical + variational calcul (Elser et al, Trugman, Sachdev)

The actual band for a single hole has minima at $q = (\pm \pi/2, \pm \pi/2)$



$$E_k = E_{min} + \frac{k_\perp^2}{2m_\perp} + \frac{k_\parallel^2}{2m_\parallel}$$

$$\chi^{\perp,\parallel} = \frac{\sqrt{m_\parallel m_\perp}}{4\pi} \quad \text{(as in 2D Fermi gas)}$$

- we should compare the scales for the effective masses and for the effective interaction between holes large U, $\Delta \gg t$

$$E_k = \Delta + \frac{2t^2}{\Delta}(\cos k_x + \cos k_y)^2$$

$$\cos k_x + \cos k_y \Big|_{\vec{k} \approx (\pi/2, \pi/2)} \sim k_\perp \Rightarrow (m_\perp)^{-1} \sim \frac{t^2}{\Delta} \sim J$$

$m_\parallel = \infty$ in mean-field. We expect $m_\parallel \sim J$
(Dagotto, Joynt, Moreo, Bacci, Gagliano)

Small U $\quad m_\perp^{-1} \sim t^2/\Delta, \quad m_\parallel \sim \frac{1}{\Delta}$

$$\tilde{\chi} \sim \sqrt{m_\perp m_\parallel} \sim \begin{cases} t^{-1}, & t \gg U \\ J^{-1}, & U \gg t \end{cases}$$

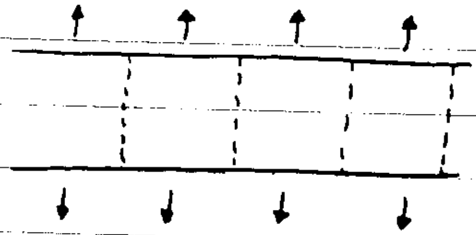
$$\Gamma^{+-} \sim \begin{cases} t, & t \gg U \\ U, & U \gg t \end{cases} \qquad \Gamma^{zz} \sim \begin{cases} t \times \left(\frac{U}{t}\right)^{1/2}, & t \gg U \\ J, & U \gg t \end{cases}$$

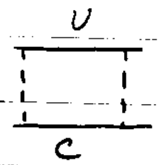
* $\bar{\chi}^{zz}$: no large parameter, which would force the instability in $\bar{\chi}^{zz}$ at low doping
* $\bar{\chi}^{+-}$: $\Gamma\tilde{\chi} \sim U/J \gg 1$ at large U

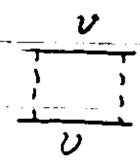
The improvements on the mean-field theory still suggest immediate instability in $\bar{\chi}^{+-}$

Caution: we have a situation when the coupling is much larger than the bandwidth $\Rightarrow$ inherently strong coupling situation $\Rightarrow$ strong vertex + self-energy correctio[ns]

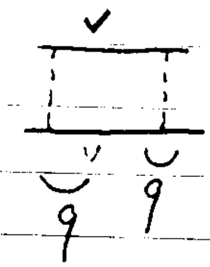
- diagramatic language:



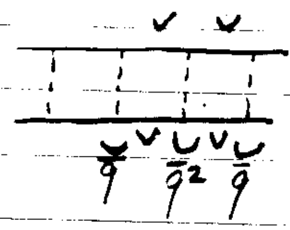




$| \equiv U \times$ (coherence factors)

$\bar{q} \sim$  $\sim \bar{q}$

$(\vec{\bar{q}} = \vec{q} - \vec{Q})$

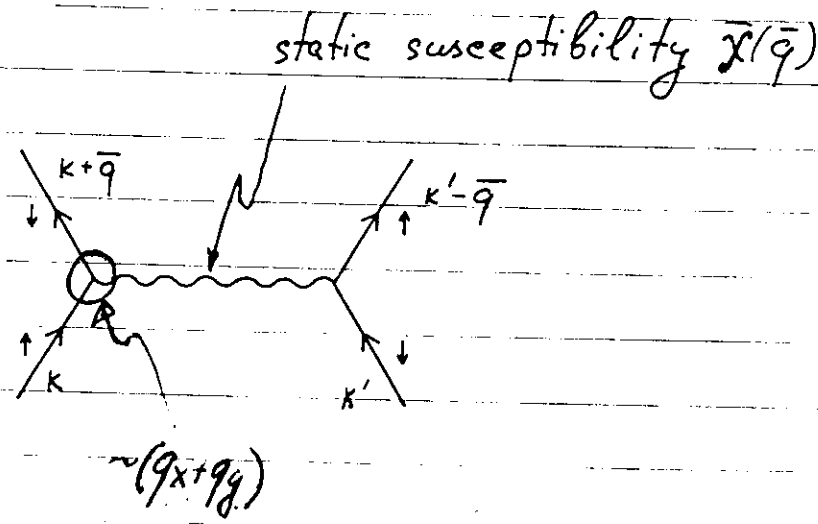
 $\sim \bar{q}^4$

* low $\bar{q}$: "valence-valence" bubbles should be separated by subsequencies of "valence-conduction" ones

* each subsequence $\equiv$ susceptibility at half filling

* dominant interaction between valence fermions is an exchange of spin waves

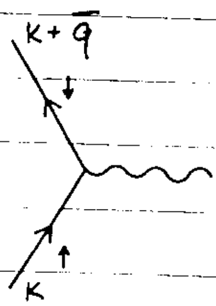
$\Gamma^{+-} =$



$$\Gamma^{+-} = \Gamma \times \left(\frac{q_x \sin k_x + q_y \sin k_y}{|q|}\right)^2$$

$$\Gamma \sim \begin{cases} t, & t \gg U \\ U, & U \gg t \end{cases}$$

3b



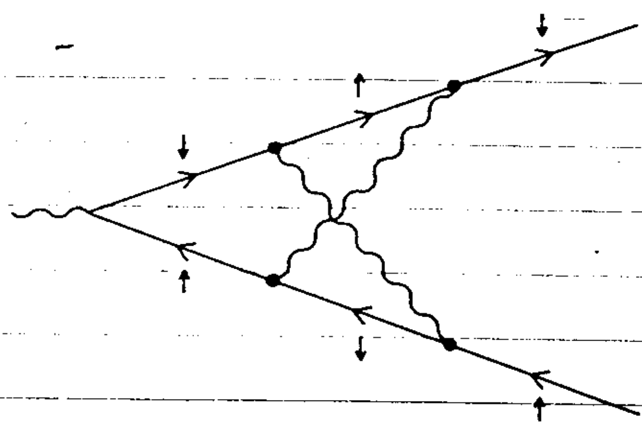
$$\Phi(k, \bar{q}) = U\left(v_{k+\bar{q}}\, u_k - u_{k+\bar{q}}\, v_k\right)$$

$$u_k = \left[\frac{1}{2}\left(1 + \varepsilon_k / E_k\right)\right]^{1/2} ; \quad v_k = \left[\frac{1}{2}\left(1 - \frac{\varepsilon_k}{E_k}\right)\right]^{1/2}$$

$$\Phi = U \, \frac{\varepsilon_k - \varepsilon_{k+\bar{q}}}{2\sqrt{E_k E_{k+\bar{q}}}} \quad ; \quad E_k \sim \Delta \sim U$$

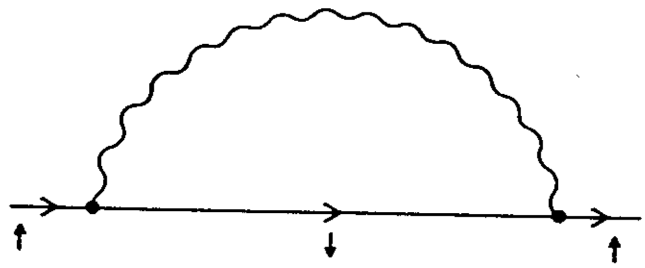
$$\left.\begin{array}{l} \Phi \sim t\,(q_x + q_y) \\ \chi \sim \dfrac{1}{J q^2} \end{array}\right\} \quad \Phi^2 \chi \sim \frac{t^2}{\underbrace{J}_{U}} \, \frac{(q_x + q_y)^2}{q^2}$$

3C



$$\Delta \Phi \sim \left(\frac{t}{\gamma}\right)^4$$

4b



$$G = \frac{Z}{\omega - E + i\delta}, \quad \delta Z \sim \left(t/J\right)^2$$

4a

- a way to proceed is to look for effective theory which will describe the system at the scales $\sim \underset{=}{O}(J)$

* $\Phi(\bar{q}) \sim (\bar{q}_x + \bar{q}_y)$
* frequency dependence is unlikely to be singular
* $\Phi(q) = \lambda\,(\bar{q}_x + \bar{q}_y)$
* the physically relevant coupling at low energies: $\boxed{\Phi^R = \Phi \times Z^2}$

* we observe, that with $\Phi^R \sim J$, the corrections become of the order of unity $\Rightarrow$ low energy theory becomes "self-consistent", it does not generate new energy scales.

$\Gamma^{+-} \sim J$ at $U \gg t$ (Shraiman & Siggia)

(Kane, Lee & Read)

$$\Phi \sim t \;,\quad Z \sim J/t \;\Rightarrow\; \Phi^R \sim t \times J/t \sim J$$

- finaly $\Gamma^{+-} \sim J$, $\Gamma^{zz} \sim J$ (or less)

- still $\Gamma\chi = \dfrac{\Gamma m_\perp}{2\pi}\sqrt{m_\parallel/m_\perp}$

$m_\perp \sim 1/J \Rightarrow \Gamma m_\perp = O(1)$. However, $\frac{m_\parallel}{m_\perp}$ well may be $\gg 1$

⊛ Final argument

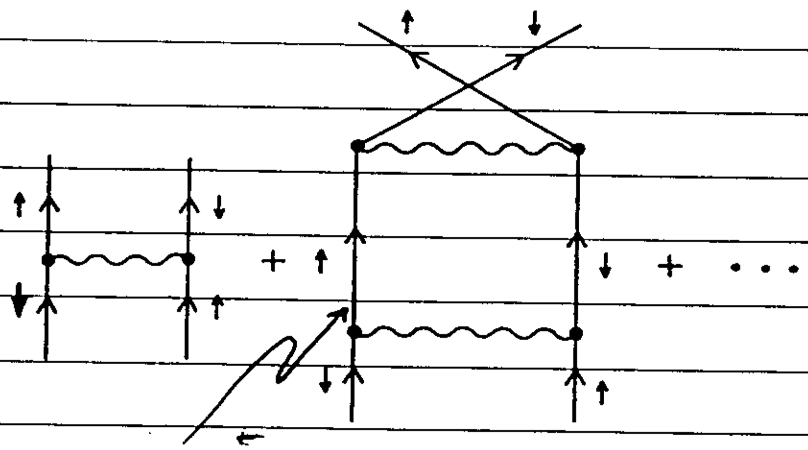
- $\Gamma\chi$ is a constant even at arbitrary small ε_F

- This is true in 2D only within the Hartree - Fock approach

- Actually, no discontinuity in $\Gamma\chi$, when the vacuum renormalization is taken into account

- $\Gamma \to T$ (scattering amplitude)

$$T^{+-} = \frac{\Gamma^{\pm}}{1 + \frac{\Gamma^{+-}}{4\pi}\sqrt{m_\parallel m_\perp}\,\ln\frac{W_0}{\omega}}$$



$$\int \frac{d^2p}{\varepsilon_p} \sim \int \frac{d^2p}{p^2} \sim \ln \ldots$$

5

$$\Gamma^{+-}\chi^{+-} \sim \frac{2}{\ln \frac{\omega_0}{\omega}} \ll 1$$

$$\omega_0 \sim \begin{cases} \Delta, & t \gg U \\ J, & U \gg t \end{cases}$$

- no instability at sufficiently small concentration of holes

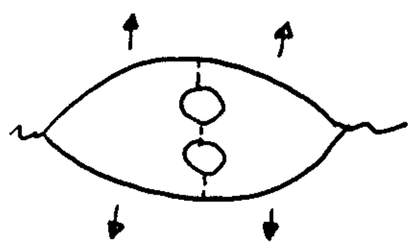
- at larger doping - <u>no pockets</u>

- the instability may occur, but the theory as no large parameter which would allow ne to make definite conclusions

* "open" Fermi surface at small ε_F (if!)

- mean - field : $\chi \sim \frac{1}{\varepsilon_F}$

- vertex corrections



- after ladder summation : at small U, the instability is likely to occur in the <u>transverse</u> channel.

Dynamical susceptibility

- suppose that ρ_s changes the sign at some finite doping $\Rightarrow$ transition into a spiral phase

- conventional wisdom: $c_{sw} \to 0$ at the transition point

Here it is not the case

$$(\bar{\chi}^{+-})^{-1} \sim \omega^2 - c_{sw}^2 q^2 + \beta q^2 \times \frac{v_F^2 q^2}{v_F^2 q^2 - \omega^2}$$

$$\omega \to 0, \quad \chi^{-1} \sim c_{sw}^2 q^2 (1 - \beta / c_{sw}^2)$$

$$\omega = c_{sw} q \quad \chi^{+} \sim \omega^2 - c_{sw}^2 q^2 \Big(1 + \underbrace{\frac{\beta}{c_{sw}^2} \quad \frac{v_F^2}{c_{sw}^2}}_{\text{small correction}}\Big)$$

RPA:
$$\omega^2 = c_{sw}^2 q^2 \begin{cases} 1 + \left(\frac{U_{eff}}{3\pi^2 J}\right)\left(\frac{\varepsilon_F}{t}\right)\left(1 + 4\sin^4 2\varphi\right), & u \gg \\ 1 + \left(\frac{4\sqrt{\pi}}{3}\right)\left(t/u\right)^{1/2}\left(\frac{\varepsilon_F}{t}\right)\left(1 + \frac{1}{4}\sin^4 2\varphi\right), & t \gg u \end{cases}$$

angular dependence: the holes mediate dipolar interactions between the spins

* <u>model</u> : pockets near $(\frac{\pi}{2}, \frac{\pi}{2})$ + T (scattering amplitu

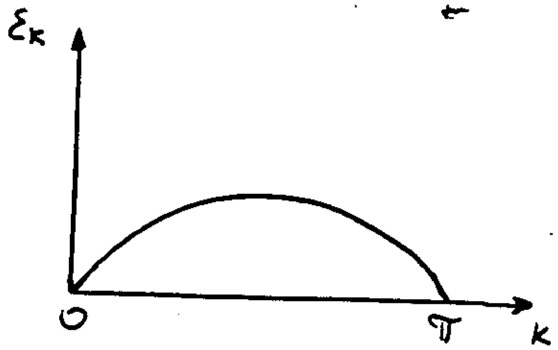
$$(\bar{\chi}^{+-})^{-1} \sim q^2 \frac{mT}{2\pi}\left(\frac{2\pi - mT}{mT} + \sqrt{\frac{\delta^2}{\delta^2-1}}\right)\Big|_{\text{at } \omega \ll c_{sw} q}$$

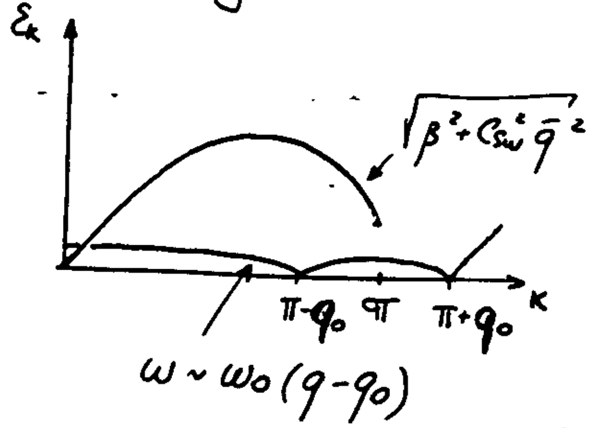
$$\delta^2 = \frac{\omega^2 m^2}{q^2 k_F^2}$$

$mT < 2\pi$ — no poles

$mT > 2\pi$: $\omega^2 = \omega_0^2 = \ominus \frac{q^2 k_F^2}{m^2}\left(\frac{mT}{2\pi} - 1\right)^2$

instability





* $\omega_0 \to 0$ at the transition (Gan, Andrei & Coleman / Shraiman & Siggia)

* the residue of the pole scales as $|\omega_0|$ and neutralizes the smallness of the spin-wave velocity near q_0

Conclusions

i) no immediate instability of AFM state upon doping

ii) the instability may occur at larger doping concentrations, but its possibility is related only to the interplay of numerical factors

iii) the first instability is likely to occur in the transverse channel <u>both</u> at $U \ll t$ and $U \gg t$

iiii) the instability is governed not by spin waves, but by collective fermionic excitations coupled to the spin background

* <u>superconductivity</u>

longitudinal channel - attraction (SWE)

transverse channel ($\Phi^2 \chi = const(q)$) - repulsion, which always (for $U \gg t$ and $t \gg U$) overshadows the attraction due to longitudinal fluctuations

this happens as long as AFM ordering is well defined