An approach towards antiferromagnetism and d-wave superconductivity in the Hubbard model

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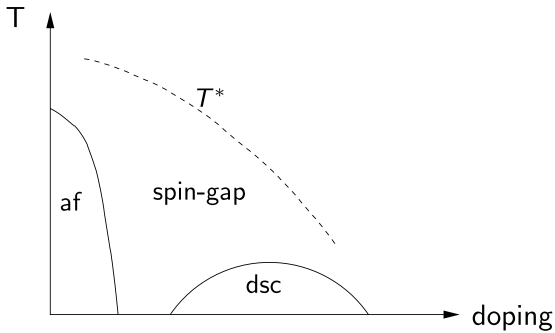
Outline

Introduction (1)

Generic phase diagram of a cuprate superconductor:



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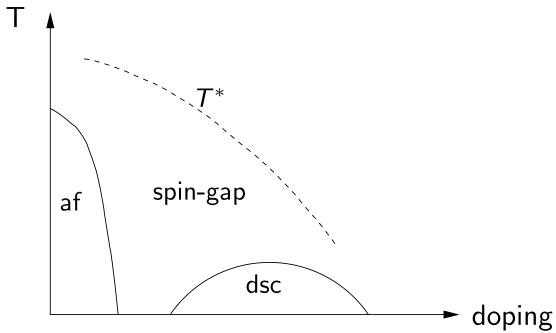

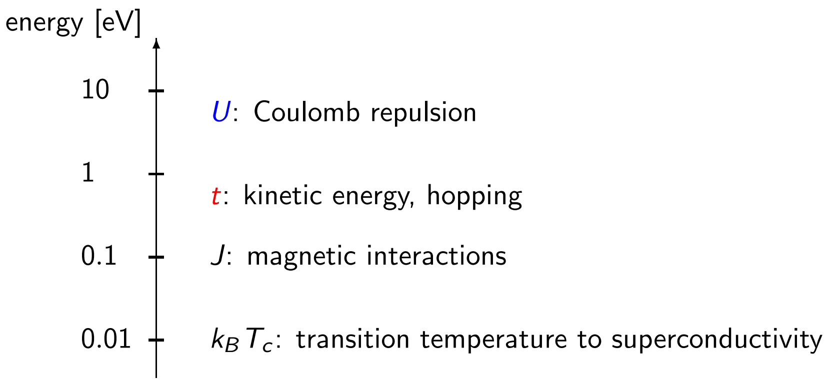

Introduction (2)

- Effective single-band model for $\mathrm{CuO_2}$-planes in HTCS:
  2d Hubbard model [e.g. Anderson '87; Zhang, Rice '88]

- 2d Hubbard model resembles important features of these materials:
  Antiferromagnetic insulator at half-filling (provided t' is not too large)
  Expected to become a d-wave superconductor away from half-filling [e.g. Scalapino '95]

- Antiferromagnetic spin wave exchange is proposed as mechanism leading to d-wave superconductivity [e.g. Miyake et. al. '86; Scalapino et. al. '86; Bickers et. al. '87]

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- "Hopping" interaction t_{ij} between neighboring lattice sites.
  ($\rightarrow$ propagation of the electrons.)

$$\Rightarrow \quad \hat{H} = \sum_{i,j,\sigma} t_{ij} \hat{\psi}^{\dagger}_{i,\sigma} \hat{\psi}_{j,\sigma} + U \sum_{i} \hat{\psi}^{\dagger}_{i,\uparrow} \hat{\psi}^{\dagger}_{i,\downarrow} \hat{\psi}_{i,\downarrow} \hat{\psi}_{i,\uparrow}$$

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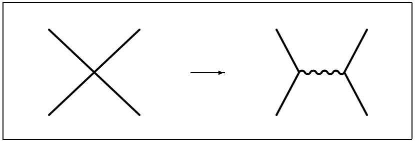
- Fermionic FRG [Zanchi, Schulz; Halboth, Metzner; Honerkamp, Salmhofer, Rice; Wegner; Kampf, Katanin;...]
  Detect antiferromagnetic and *d*-wave superconducting instabilities, antiferromagnetic fluctuations trigger coupling in the *d*-wave pairing channel,...
- FRG in partially bosonized formulations: Interaction between electrons mediated by boson exchange.



  Well-suited to study collective effects and spontaneous symmetry breaking.
- Temperature dependence of antiferromagnetic order close to half filling studied in [Baier, Bick, Wetterich '04].
- We propose an effective coarse grained model for the Hubbard model which is based on the exchange of antiferromagnetic and *d*-wave collective bosons [HCK, Müller, Wetterich '08].

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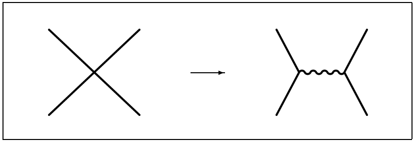

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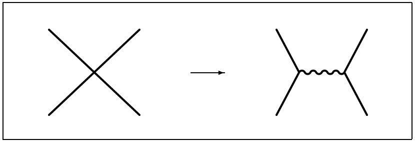

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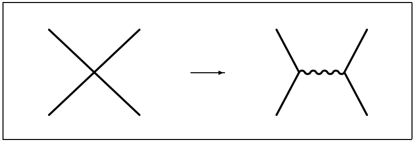

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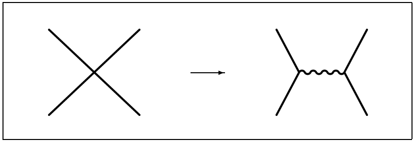

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- We investigate a bosonic field $\mathbf{a}$ which represents an antiferromagnetic fermion bilinear,

$$\mathbf{a}(X) \triangleq \psi^\dagger(X)\boldsymbol{\sigma}\psi(X)e^{i\Pi X} \quad X = (\tau, \mathbf{x}), \quad \Pi = (0, \boldsymbol{\pi} = (\pi, \pi)).$$

- Antiferromagnetic order is indicated by $\langle \mathbf{a}(X) \rangle \neq 0$.

- Simplest description of antiferromagnetism is given by

$$U_{\mathbf{a}}[\mathbf{a}] \;=\; \bar{m}_a^2 \alpha + \frac{1}{2}\bar{\lambda}_a \alpha^2, \quad \alpha = \mathbf{a}^2/2.$$

  Vanishing of $\bar{m}_a^2$ corresponds to diverging four fermion coupling,
  $\bar{m}_a^2 < 0$ leads to a minimum of $U_{\mathbf{a}}$ at $\alpha_0 \neq 0 \longrightarrow$ SSB.

- We start with a Yukawa-like ansatz for the effective average action similar as [Baier, Bick, Wetterich, 04]

$$\Gamma_k[\mathbf{a}, \psi, \psi^*] = \Gamma_{F,k}[\psi, \psi^*] + \Gamma_{\mathbf{a},k}[\mathbf{a}] + \Gamma_{F\mathbf{a},k}[\mathbf{a}, \psi, \psi^*],$$

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- Fermionic kinetic term:

$$\Gamma_{F,k} = \sum_Q \psi^\dagger(Q)\big(i\omega - \mu - 2t(\cos q_1 + \cos q_2) - 4t' \cos q_1 \cos q_2\big)\psi(Q)\,.$$

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For $U = 3U_m \longrightarrow$ equivalence to fermionic Hubbard model.

- Four fermion coupling U completely bosonized on initial scale Λ_{HM}.

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- The purely bosonic term is described by a kinetic term and a local effective potential $U_{\mathbf{a}}$

$$\Gamma_{a,k} = \frac{1}{2}\sum_Q \mathbf{a}^T(-Q)P_a(Q)\mathbf{a}(Q) + \sum_X U_{a,k}[\mathbf{a}]\,.$$

- The Yukawa like interaction term couples the bosonic field to the fermions,

$$\Gamma_{F\mathbf{a},k} = -\bar{h}_a \sum_Q \mathbf{a}(-Q)\cdot\tilde{\mathbf{a}}(Q) = -\sum_{K,Q,Q'} \delta(K + \Pi - Q + Q')\bar{h}_a\mathbf{a}(K)\cdot[\psi^\dagger(Q)\boldsymbol{\sigma}\psi(Q')]\,.$$

- Initial conditions:

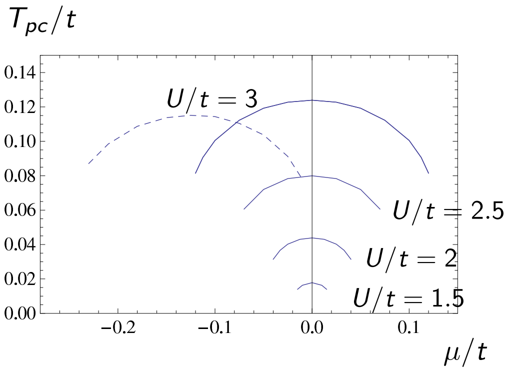
$$\bar{m}_a^2|_{\Lambda_{HM}} = U_m\,, \quad \bar{h}_a|_{\Lambda_{HM}} = U_m\,, \quad \bar{\lambda}_a|_{\Lambda_{HM}} = 0\,, \quad P_a(Q)|_{\Lambda_{HM}} = 0\,.$$

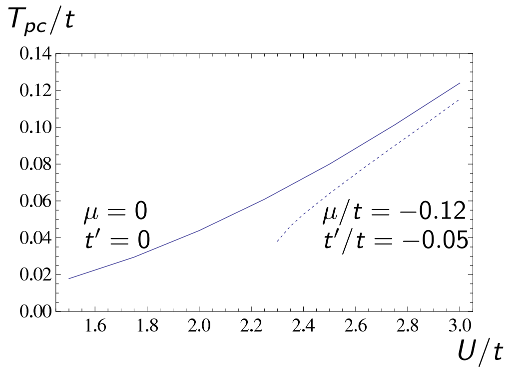
  For $U = 3U_m \longrightarrow$ equivalence to fermionic Hubbard model.

- Four fermion coupling U completely bosonized on initial scale Λ_{HM}.

Antiferromagnetism (3)

- T_{pc} as a function of μ/t and U/t ($t' = 0$, solid line; $t' = -0.05t$, dashed line):





T_{pc} is defined as highest temperature where the bosonic mass term $\bar{m}_a^2$ vanishes on a scale $k_{SSB} > 0$ in the renormalization flow.
This indicates the existence of local order for $T < T_{pc}$.
Critical temperature $T_c < T_{pc}$.

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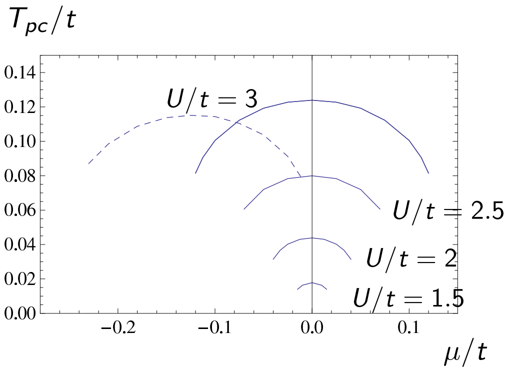

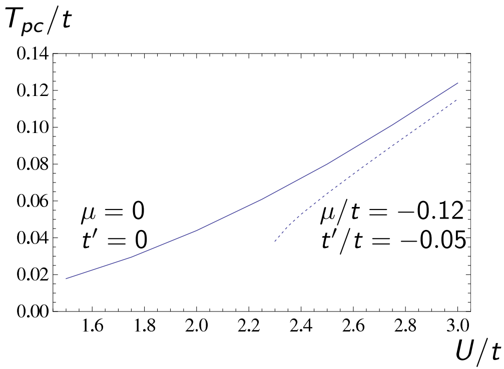

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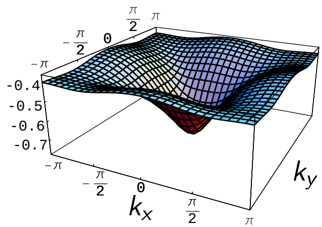
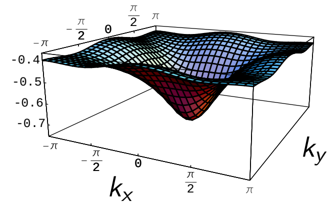
Antiferromagnetism (4)

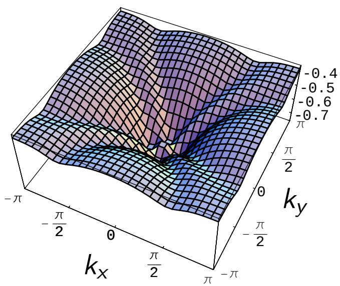
- One-loop (mean field) correction to bosonic propagator $\Delta G_a^{-1}(0, k_x, k_y)$:



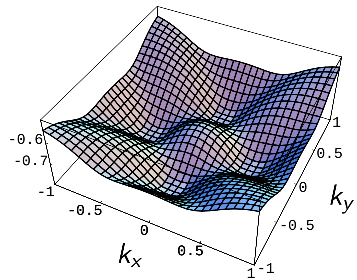
(a) $\mu = 0,\ t' = 0,\ T/t = 0.35$



(b) $\mu/t = -0.3,\ t' = 0,\ T/t = 0.3$



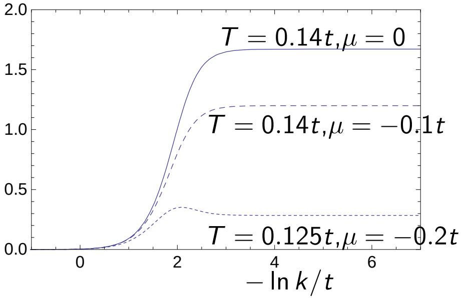
(c) $\mu/t = -0.3,\ t' = 0,\ T/t = 0.1$



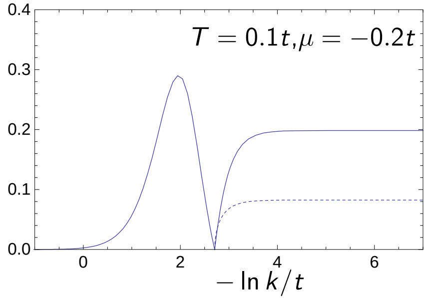
(d) $\mu/t = -0.5,\ t'/t = -0.05,\ T/t = 0.1$

Antiferromagnetism (5)

- Flow of the gradient coefficient A_a and incommensurate wave vector:



(a) A_a in commensurate situation



(b) A_a, $\hat{q}$ in incommensurate situation

d-wave pairing (1)

Introduce bosonic field d which corresponds to fermion bilinear whose expectation value describes d-wave superconductivity:

$$\tilde{d}(Q=0) = \frac{1}{2}\sum_K (\cos k_1 - \cos k_2)\psi(K)\epsilon\psi(-K)$$

$$= \quad \frac{1}{4}\Big\{\psi(X)\epsilon\psi(X+\hat{e}_1) + \psi(X)\epsilon\psi(X-\hat{e}_1) - \psi(X)\epsilon\psi(X+\hat{e}_2) - \psi(X)\epsilon\psi(X-\hat{e}_2)\Big\}\,,$$

where $\hat{e}_1$ and $\hat{e}_2$ are the unit vectors in the plane and $\epsilon = i\sigma_2$.

$\longrightarrow$ Lattice representation of a $d_{x_1^2-x_2^2}$ wave. Changes sign under rotation by 90° but not under reflection at the x_1 or x_2 axes.

For a more extensive classification, see [Scalapino 95].

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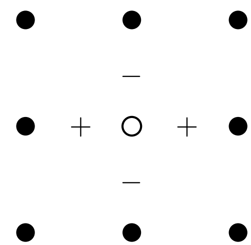
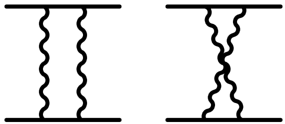


Regeneration of four fermion coupling

- Bosonization is not perfect in the sense that the four fermion coupling is regenerated by fluctuations:



$k < \Lambda_{HM}$:

$$\Gamma_4 = \frac{1}{4} \sum_{Q_1,\ldots,Q_4} \Gamma^{(4)}_{F,\alpha\beta\gamma\delta}(Q_1, Q_2, Q_3, Q_4)\delta(Q_1 - Q_2 + Q_3 - Q_4) \times \psi^*_\alpha(Q_1)\psi_\beta(Q_2)\psi^*_\gamma(Q_3)\psi_\delta(Q_4) \neq 0 \, .$$

- For spin rotation invariant systems the spin structure of the four fermion interaction has the general form:

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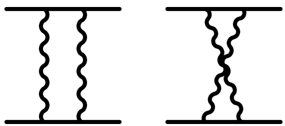

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Projection onto d-wave pairing channel (1)

- We define a momentum dependent d-wave channel coupling $\lambda_F^d(\mathbf{l},\mathbf{l}')$ by

$$\lambda_F^d(\mathbf{l},\mathbf{l}') = \frac{1}{2}\{\Gamma^{(4)}_{F,s}(L,L',-L,-L') - \Gamma^{(4)}_{F,s}(R(L),L',-R(L),-L')\}\ ,$$

with $L^{(')} = (\pi T, \mathbf{l}^{(')})$, $R(L)$ denotes a rotation of the spatial components $\mathbf{l}$ of L by 90°.

- Antiferromagnetic and other channels are subtracted in this way.

- We find that $\partial_k \lambda_F^d(\mathbf{l},\mathbf{l}')$ is well approximated by the flow of a simple d-wave channel coupling λ_F^d of the form

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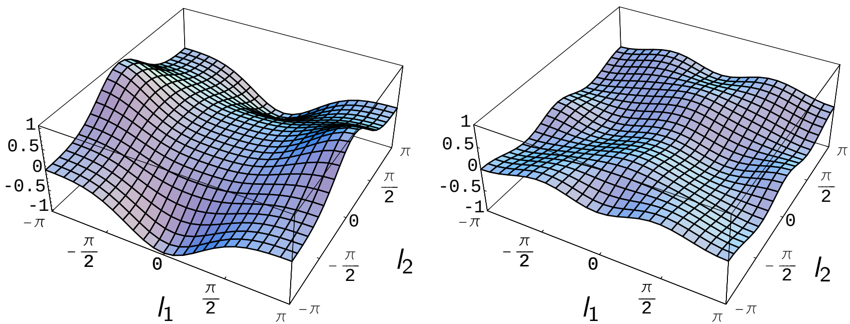
Projection onto d-wave pairing channel (2)

- In (a) we show the normalized momentum dependence of the rhs of the flow equation for the fermionic coupling $\frac{1}{4}\left(\partial_k \lambda_F^d(\mathbf{l},\mathbf{l}')/\partial_k \lambda_F^d\right)$ for $k = \Lambda_{HM}$.
  In (b) we display the residual coupling: $\frac{1}{4}\left(\partial_k \lambda_F^d(\mathbf{l},\mathbf{l}')/\partial_k \lambda_F^d - f_d(2\mathbf{l}) f_d(2\mathbf{l}')\right)$.



(a) $T/t = 0.5\,, \mu/t = -0.5$ (b) $T/t = 0.5\,, \mu/t = -0.5$

d-wave pairing (2)

- Extend truncation of effective action by

$$\Gamma_{d,k}[d,d^*] = \sum_K d^*(K) P_d(K) d(K) + \sum_X U_{d,k}[d]\,.$$

Here: $P_d(K) = 0$ and $U_{d,k}[d] = \bar{m}_d^2 d^* d$.

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$$\begin{aligned}\Gamma_{Fd,k}[\psi,\psi^*,d,d^*] &= -\bar{h}_d \sum_Q (d^*(Q)\tilde{d}(Q) + d(Q)\tilde{d}^*(Q)) \\ &= -\frac{\bar{h}_d}{2} \sum_{K,Q,Q'} \delta(K-Q-Q') f_d(\mathbf{q}-\mathbf{q}') \\ &\quad \times \left(d^*(K)[\psi^T(Q)\epsilon\psi(Q')] - d(K)[\psi^\dagger(Q)\epsilon\psi^*(Q')] \right),\end{aligned}$$

which couples the d-field to the fermions. The d-wave form factor is

$$f_d(\mathbf{q}) \equiv \cos\frac{q_1}{2} - \cos\frac{q_2}{2}\,.$$

Only the Yukawa coupling $\bar{h}_d$ depends on scale k (within our approximation).

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- Idea: Make the bosons "perfect" on all scales [Gies, Wetterich 02; Pawlowski 07]. We redefine the bosonic fields $(\mathbf{a}, d, d^*) \to (\mathbf{a}_k, d_k, d_k^*)$ such that the on scale k regenerated four fermion coupling can be bosonized.
- In general:

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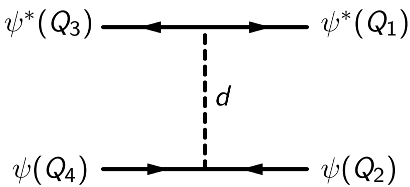
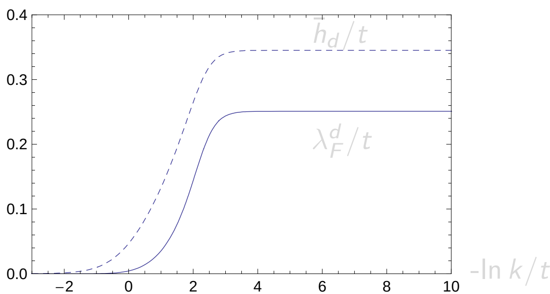
- Effective four fermion interaction in the d-wave pairing channel mediated by d-boson exchange:



$$\lambda^d_{F,\mathrm{eff}}(Q_1, Q_2, Q_3, Q_4) = \frac{\bar{h}_d^2}{\bar{m}_d^2} f_d(\mathbf{q}_1 - \mathbf{q}_3) f_d(\mathbf{q}_2 - \mathbf{q}_4) \delta(Q_1 - Q_2 + Q_3 - Q_4)\,.$$

- Flow of the four fermion coupling in the d-wave channel λ_F^d and the Yukawa coupling $\bar{h}_d$:

$(T/t = 0.13,$
$\mu/t = -0.1,$
$t' = 0)$



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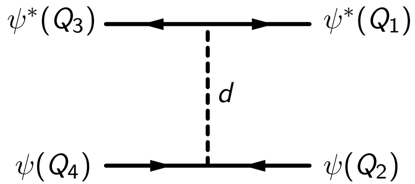
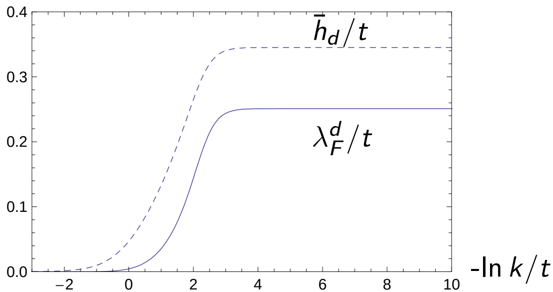


$$\lambda^d_{F,\mathrm{eff}}(Q_1, Q_2, Q_3, Q_4) = \frac{\bar{h}_d^2}{\bar{m}_d^2} f_d(\mathbf{q}_1 - \mathbf{q}_3) f_d(\mathbf{q}_2 - \mathbf{q}_4)\delta(Q_1 - Q_2 + Q_3 - Q_4)\,.$$

- Flow of the four fermion coupling in the d-wave channel λ^d_F and the Yukawa coupling $\bar{h}_d$:

$(T/t = 0.13,$
$\mu/t = -0.1,$
$t' = 0)$



Outlook

- Study influence of d-boson exchange on antiferromagnetism. Mutual influence of both bosonic fluctuations.
- Investigate role of incommensurate antiferromagnetic fluctuations, ferromagnetism and spontaneous deformations of Fermi surface (Pomeranchuk instabilities).
- Study region where d-wave coupling dominates below a certain scale

  $\longrightarrow$ Calculate T_{pc} for d-wave superconductivity

  $\longrightarrow$ Phase transition to d-wave superconductivity
- Competition between antiferromagnetic order and d-wave superconductivity depending on the doping.
  $\longrightarrow$ Temperature dependence of antiferromagnetic order and d-wave superconductivity.
- Different universality classes at $T = 0$.

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