Flow Equations of Hamiltonians

Application to the Hubbard Model

http://www.tphys.uni-heidelberg.de/~statphys/floweq.html

- Basic idea and method

  Continuous unitary transformation (as function of the "flowparameter" ℓ) for Hamiltonians, which makes off-diagonal matrix elements decrease.

  Annalen der Physik 3 (Jan. '94) 77–91

  For renormalization of ultra-violett divergencies: Similarity renormalization S. D. Glazek, K. G. Wilson, Phys. Rev. D48 (Dec. '93) 5863; PRD 49 ...

- Elimination of the electron-phonon interaction

  P. Lenz + F.W., A. Mielke, M. Ragwitz

- Possible Phases of the 2D-Hubbard model

  I. Grote, V. Hankevych, F.W.

Application of Flow Equations to

n-orbital model of interacting electrons
$n \to \infty$ closed equations F.W.

Luttinger model
C.P. Heidbrink, G.S. Uhrig

Elimination of electron-phonon interaction
P. Lenz, A. Mielke, M. Ragwitz, F.W.

Anderson-Impurity Model
S. Kehrein, A. Mielke

Spin-Boson Model
S. Kehrein, A. Mielke, P. Neu, T. Stauber

Light Front QCD and QED
S. Glazek, K. Wilson, T. Walhout, A. Harindranath, W. Zhang, R. Perry, B. Jones, M. Brisudova, HC. Pauli, E. Gubankova

Hubbard-Model (Strong Coupling), Heisenberg Antiferromagnet
J. Stein

Lipkin-Model
A. Mielke, H.J. Pirner, B. Friman, J. Stein

Kondo-Model
E. Vogel, W. Hofstetter, S. Kehrein, C. Slezak, Th. Pruschke, M. Jarrell

Spin-Peierls, dimerized Spin-chains
G. Uhrig, C. Knetter, C. Raas, A. Bühler

Spin-Quadrumers
W. Brenig, A. Honecker

Sine-Gordon-Model
S. Kehrein

Boson-Fermion-Systems
T. Domanski, J. Ranninger

Hubbard-Model (Weak Coupling)
I. Grote, V. Hankevych, F.W.

Dirac particle in External Potential
A. Bylev, H.J. Pirner

Contact-Potential in 2 Dimensions
S. Glazek, J. Mylnik

Quantum chemistry: Water molecule
S.R. White

International Workshop on
Functional Renormalization in Interacting
Quantum Many-Body Problems

Max-Planck-Institut für Physik komplexer Systeme
Dresden, March 10-21, 2003
http://www.mpipks-dresden.mpg.de/ ˜friqus03
Deadline for application is November 15, 2002

Scientific coordinators:

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E. Fradkin (Urbana)	J. Fröhlich (ETH Zürich)	M. Imada (Tokyo)
A. Luther (Nordita)	V. Meden (Göttingen)	W. Metzner (Stuttgart)
T.M. Rice (ETH Zürich)	M. Salmhofer (Leipzig)	H. Schoeller (Aachen)
K. Schönhammer (Göttingen)	R. Shankar (Yale)	C.M. Varma (Bell Labs/Lucent)

Basic idea and method

F. W., Annalen der Physik 3 (1994) 77

$$H(\ell) = \mathcal{U}(\ell)\, H\, \mathcal{U}^+(\ell)$$

$$\frac{dH}{d\ell} = [\eta(\ell), H(\ell)] \qquad \eta(\ell) = \frac{d\mathcal{U}(\ell)}{d\ell}\mathcal{U}^+(\ell) = -\eta^+(\ell)$$

Example:

$$H = \begin{pmatrix} \varepsilon_1 & h \\ h^* & \varepsilon_2 \end{pmatrix} \qquad \eta = \begin{pmatrix} 0 & a \\ -a^* & 0 \end{pmatrix}$$

$$[\eta, H] = \begin{pmatrix} ah^* + ha^* & (\varepsilon_2 - \varepsilon_1) a \\ (\varepsilon_2 - \varepsilon_1) a^* & -ah^* - ha^* \end{pmatrix}$$

Choice: $a = (\varepsilon_1 - \varepsilon_2) \cdot h$

$$\frac{dh}{d\ell} = -(\varepsilon_1 - \varepsilon_2)^2 \cdot h$$

$$r^2 := |h|^2 + \left(\frac{\varepsilon_1 - \varepsilon_2}{2}\right)^2$$

$$|h(\ell)|^2 = \frac{|h(0)|^2 r^2 e^{-8r^2\ell}}{\underbrace{r^2 - |h(0)|^2} + |h(0)|^2 e^{-8r^2\ell}}$$

General:

$$\eta_{kk'} = (\varepsilon_k - \varepsilon_{k'})\, h_{kk'}$$

$$\frac{dH}{d\ell} = [\eta, H], \qquad \eta^+ = -\eta$$

$$\eta_{kk'} = (\varepsilon_k - \varepsilon_{k'})\, h_{kk'} \qquad \eta = [H_d, H]$$

$$\frac{\partial h_{kk'}}{\partial \ell} = \sum_{k''} (\varepsilon_k + \varepsilon_{k'} - 2\varepsilon_{k''})\, h_{kk''} h_{k''k'}$$

$$\frac{d}{d\ell} \sum_{\substack{k,k' \\ k \neq k'}} h_{kk'} h_{k'k} = -\frac{d}{d\ell} \sum_k \varepsilon_k^2$$

$$= -2 \sum_{k,k'} (\varepsilon_k - \varepsilon_{k'})^2 h_{kk'} h_{k'k}$$

Example:

$$\varepsilon_k \sim k, \quad h_{kk'} = h_{k-k'} \qquad (k \neq k')$$

$$h_{kk'}(\ell) = h_{kk'} \cdot \exp\left(-(\varepsilon_k - \varepsilon_{k'})^2 \ell\right)$$

$$[\ell] = \frac{1}{\text{energy}^2}$$

Basis states of $H(\ell)$ have an energy width

$$\Delta E \sim O\left(\frac{1}{\sqrt{\ell}}\right)$$

Elimination of Electron-Phonon Interaction

FW + P. Lenz, Nucl. Phys. B 482 ('96) 693

$$H = H^d + H^r = H^0 + V + H^r$$

$$H^0 = \sum \omega_q a_q^+ a_q + \sum \epsilon_k :c_{ks}^+ c_{ks}:$$

(↑ phonons, ↑ electrons)

$$V = \sum V_{kk'q} :c^+_{k+q\,s} c^+_{k'-q\,s'} c_{k's'} c_{ks}: \qquad \text{el-el.-interaction}$$

$$H^r = \sum M_{kq}\, a^+_{-q} c^+_{k+q\,s} c_{ks} + \text{h.c.} \qquad \text{el-phon.-interact.}$$

$$\eta = [H^d, H] = [H^d, H^r] \approx [H^0, H^r]$$

$$= \sum M_{k,q} \underbrace{(\epsilon_{k+q} - \epsilon_k + \omega_q)}_{\alpha_{k,q}} a^+_{-q} c^+_{k+q\,s} c_{ks} - \text{h.c.}$$

$$\frac{dH}{dl} = [\eta, H] \approx [\eta, H^0] + [\eta, H^r]$$

$$[\eta, H_0] = -\sum \alpha_{kq}^2 M_{k,q}\, a^+_{-q} c^+_{k+q\,s} c_{ks} + \text{h.c.}$$

$$\frac{d M_{k,q}(l)}{dl} = -\alpha_{k,q}^2 M_{k,q}(l)$$

$$M_{k,q}(l) = M_q(0) \exp(-\alpha_{k,q}^2 l)$$

$$[\eta, H^r] = -\sum (\alpha_{k,q} + \alpha_{k'-q,q}) M_{k,q} M^*_{k'-q,q} :c^+_{k+q\,s} c^+_{k'-q\,s'} c_{k's'} c_{ks}: + \ldots$$

$$\frac{d V_{k,k',q}(l)}{dl} = -(\alpha_{k,q} + \alpha_{k'-q,q}) M_{k,q}(l) M^*_{k'-q,q}(l)$$

$$V_{kk'q}(\infty) = V_{kk'q}(0) - \frac{\alpha_{kq} + \alpha_{k'-q,q}}{\alpha_{kq}^2 + \alpha_{k'-q,q}^2} |M_q(0)|^2$$

$$V_{k,-k,q}(\infty) = V_{k,-k,q}(0) - |M_q(0)|^2 \frac{\omega_q}{\omega_q^2 + (\epsilon_{k+q} - \epsilon_k)^2}$$

Fröhlich (1952) obtained − sign.

Effective interaction without pole also obtained by similarity renormalization (A. Mielke)

Similar for Schrieffer-Wolff transformation (S. Kehrein, A. Mielke)

Both methods yield same result for $V_{kk'q}$, if $\epsilon_{k+q} + \epsilon_{k'-q} = \epsilon_{k'} + \epsilon_k$ (on-shell).

Perturbation theory between blocks is not unique, since it is only determined up to unitary transformations within the blocks.

T_c calculated from the effective interaction are numerically in good agreement with Eliashberg and related theories (MacMillan & Dynes) (A. Mielke).

Flow equations do not introduce retarded interactions, but keep the interaction instantaneous.

Asymptotics of $\omega_q(\ell)$

$$\frac{d\omega_q(\ell)}{d\ell} = 2\sum_k |M_{k,q}(\ell)|^2 \alpha_{k,q}(\ell)\,(n_{k+q} - n_k)$$

$$M_{k,q}(\ell) = M_q \cdot e^{-\int_0^\ell d\ell' \alpha_{k,q}^2(\ell')}$$

$$\alpha_{k,q}(\ell) = \varepsilon_{k+q} - \varepsilon_k + \omega_q(\ell)$$

asymptotically

$$\omega_q(\ell) = \omega_q(\infty) + \frac{1}{2\sqrt{\ell_0(q)+\ell}}$$

$$\Rightarrow M_{k,q}(\ell) = M_q \cdot \left(\frac{\ell_0(q)}{\ell+\ell_0(q)}\right)^{1/4} \times$$

$$\times e^{-\alpha_{kq}^2(\infty)\ell - 2\alpha_{kq}(\infty)\left(\sqrt{\ell_0(q)+\ell} - \sqrt{\ell_0(q)}\right)}$$

$$\ell_0(q) = \frac{1}{\left(V M_q^2 \frac{m^2}{q}\,\omega_q(\infty)\,\frac{\sqrt{2}}{\pi^{3/2}}\,e^2\right)^2} \propto \frac{1}{q^2}$$

Equation for $\varepsilon_k(\ell)$:

$$\frac{d\varepsilon_k(\ell)}{d\ell} = -\sum_q |M_{k,q}(\ell)|^2 \alpha_{k,q}(\ell)\,(1 - n_{k+q})$$

$$+ \sum_q |M_{k+q,-q}(\ell)|^2 \alpha_{k+q,-q}(\ell)\, n_{k+q}$$

Possible Phases of the Hubbard-Modell

I. Grote, E. Körding, F.W.
J. Low Temp. Physics 126 (2002)
cond-mat/0106604

V. Hankevych, I. Grote, F.W.
Phys. Rev. B (Oct. 2002)
cond-mat/0205213

V. Hankevych, F. W.
cond-mat/0207612

Gradient Procedure

$G(H)$ shall be minimized, e.g.

$$G(H) = \frac{1}{2} \sum g_{ij,kl} H_{ji} H_{lk}$$

$G(H)$ real $\rightarrow$ $dG = 2 \frac{\partial G}{\partial H_{ij}} dH_{ij}$ real $\rightarrow$ $\frac{\partial G}{\partial H}$ hermitean

$\uparrow$ $\left(\frac{\partial G}{\partial H}\right)_{ji}$

$$\frac{dG}{dl} = \mathrm{tr}\left(\frac{\partial G}{\partial H} [\eta, H]\right) = \mathrm{tr}\left(\eta \underbrace{\left[H, \frac{\partial G}{\partial H}\right]}_{\text{antihermitean}}\right)$$

$$\eta := \left[H, \frac{\partial G}{\partial H}\right]$$

$\uparrow$ H^r

Example

$H^r = [v,[v,H]]$ — v hermitean: number of phonons, number of quasi-particles

$$G = -\frac{1}{2} \mathrm{tr}\left(([v,H])^2\right)$$

Linear G (Mielke, Stein)

$(H_r)_{ij} = -j\,\delta_{ji}$ $\qquad \eta_{ji} = (i-j) H_{ji}$

$$G = -\sum_k k H_{kk}$$

orders states in increasing order of energies.

Choose

$$H_r = \sum_\alpha [v^\alpha, [v^\alpha, H]]$$

with

$$v^\alpha = \sum_k v_k^\alpha c_k^+ c_k, \qquad v_k^\alpha = v_{k+q_0}^\alpha = -v_{-k}^\alpha$$

Then we keep antiferromagnetic (wave-vector q_0) and pair-interactions.

$$H = \sum \varepsilon_q :c^+_{qs} c_{qs}: + \frac{1}{2\Omega} \sum V(k_1,k_2,q_1,q_2) :c^+_{k_1 s_1} c_{q_1 s_1} c^+_{k_2 s_2} c_{q_2 s_2}:$$

$$\Rightarrow H^r = \frac{1}{2\Omega} \sum r(k_1,k_2,q_1,q_2) V(k_1,k_2,q_1,q_2) :c^+ c c^+ c:$$

$$r(k_1,k_2,q_1,q_2) = \sum_\alpha \left(v^\alpha_{k_1} + v^\alpha_{k_2} - v^\alpha_{q_1} - v^\alpha_{q_2}\right)^2$$

First order in U:

$$V^{(1)}(l) = U e^{-r(\Delta\varepsilon)^2 l}$$

Application to Hubbard-Model

Starting from the Hubbard-model

$$H(0) = -\sum_k (2t(\cos k_x + \cos k_y) + 4t' \cos k_x \cos k_y) c_k^\dagger c_k + \frac{U}{N} \sum c_k^\dagger c_q^\dagger c_{q-p} c_{k+p} \quad (5)$$

we perform the calculation in second order in U and obtain a Hamiltonian

$$\begin{aligned} H(\infty) &= \sum_k \epsilon_k c_k^\dagger c_k \\ &+ \frac{1}{N} \sum V_{\mathrm{B}}(k,q) : c_k^\dagger c_{-k}^\dagger c_{-q} c_q : \\ &+ \frac{1}{N} \sum V_{\mathrm{HF}}(k,q) : c_k^\dagger c_q^\dagger c_q c_k : \\ &+ \frac{1}{N} \sum V_{\mathrm{AC}}(k,q) : c_k^\dagger c_q^\dagger c_{q-q_0} c_{k+q_0} : \\ &+ \frac{1}{N} \sum V_{\mathrm{Y}}(k,q) : c_k^\dagger c_{q_0-k}^\dagger c_{q_0-q} c_q :, \quad (6) \end{aligned}$$

for which molecular-field approximation is exact.

Order-Parameter

Particle-particle $\Psi(k) = < c_k^\dagger c_{-k}^\dagger >$, $< c_k^\dagger c_{q_0-k}^\dagger >$

Particle-hole homogeneous $\nu(k) = < c_k^\dagger c_k >$, $< c_k^\dagger c_{q_0+k} >$.

$3 \times 3 \times 5$ Symmetries

	particle-particle	particle-hole S=0	particle-hole S=1
homogeneous	Superconductivity d_+	Pomeranchuk-instability $d_{+,-}$	Ferromagnetism s_+
$\Psi(k) = \Psi(q_0 - k)$ $\nu(k) = \nu(k + q_0)$			Antiferromagnetism s_+
$\Psi(k) = -\Psi(q_0 - k)$ $\nu(k) = -\nu(k + q_0)$		Flux-phases d_+ Band-Splitting p	Flux-phases d_+

s_+, $s_- = g_{xy(x^2-y^2)}$, $d_+ = d_{x^2-y^2}$, $d_- = d_{xy}$, $p = p_x$, p_y.

Instabilities

We expand the free energy F to second order in possible order-parameters $\Psi_k =< c_k^\dagger c_{-k}^\dagger >$, $< c_k^\dagger c_k > - < c_k^\dagger c_k >_0$, $< c_k^\dagger c_{q_0+k} >$, $< c_k^\dagger c_{q_0-k}^\dagger >$,

$$\beta F = \beta E - S$$

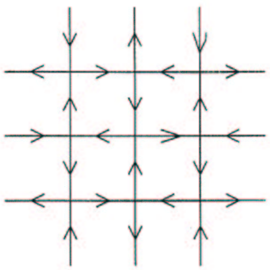
$$= \frac{1}{N}\sum(\beta U)(1+\frac{U}{t}V_{k,q})\Psi_k^*\Psi_q + \sum_k f_k \Psi_k^* \Psi_k$$

$$= \sum\left(\frac{U}{t}A_{k,q} + \left(\frac{U}{t}\right)^2 B_{k,q} + \delta_{k,q}\right)\sqrt{f_k}\Psi_k^*\sqrt{f_q}\Psi_q. \tag{7}$$

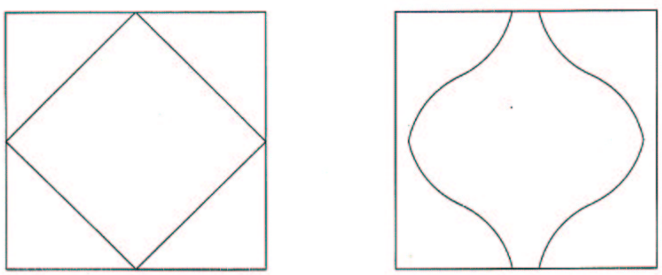
Determination of the critical values $(U/t)_c$, for which $(U/t)A + (U/t)^2 B$ has an eigenvalue -1. Instability with respect to the corresponding order-parameter.

Selection of possible Phases

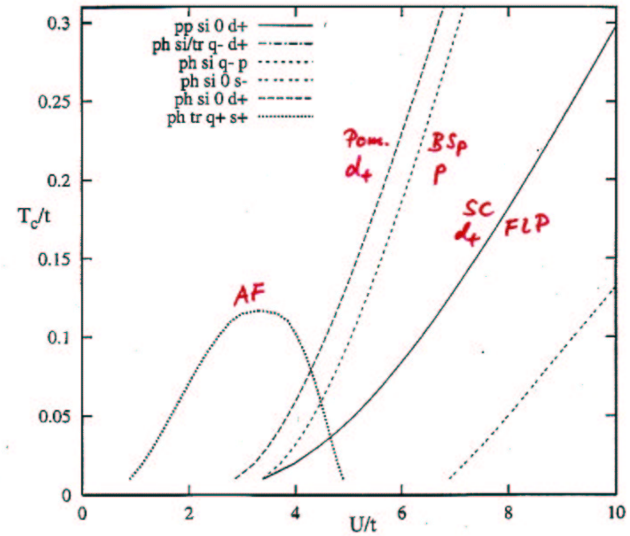
AF	Antiferromagnetism	ph	tr	q_+	s_+
Pom	Pomeranchuk Inst.	ph	si	0	d_+, $s_+ \to g_+$, $d_- \to i_-$
SC	Superconductivity	pp	si	0	d_+
FLP	Flux-Phase	ph	si / tr	q_-	d_+
BSp	Band-Splitting	ph	si	q_-	p
Ms*	Magnetic	ph	tr	0	s_+
Mp	"	ph	tr	0	p



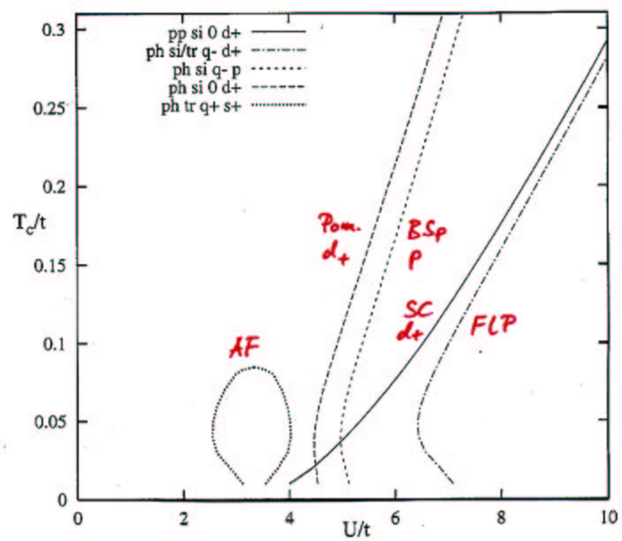
Imaginary part of hopping terms in Flux-Phases



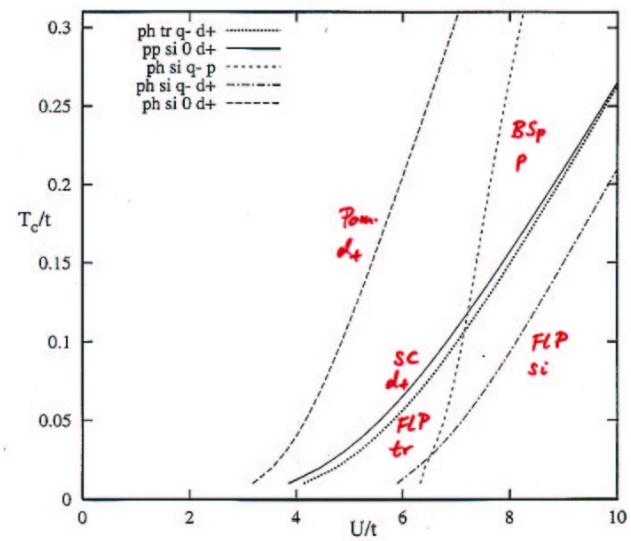
Deformation of the Fermi edge for d_+-wave Pomeranchuk instabilities (at half filling)



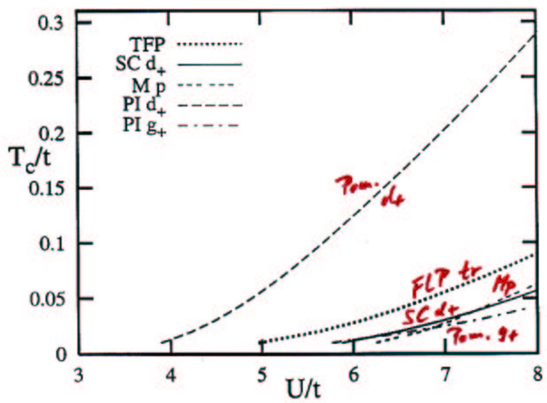
$t' = 0, \quad n = 1.00, \quad \mu = 0.$



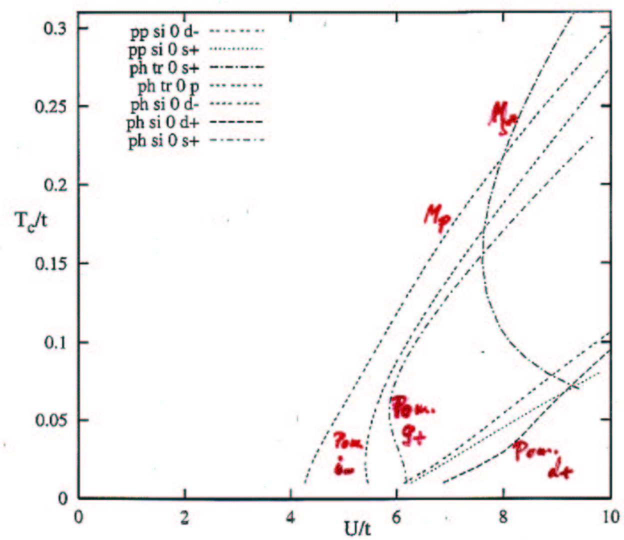
$t' = 0, \quad n = 1.06, \quad \mu/t = 0.097...0.146.$



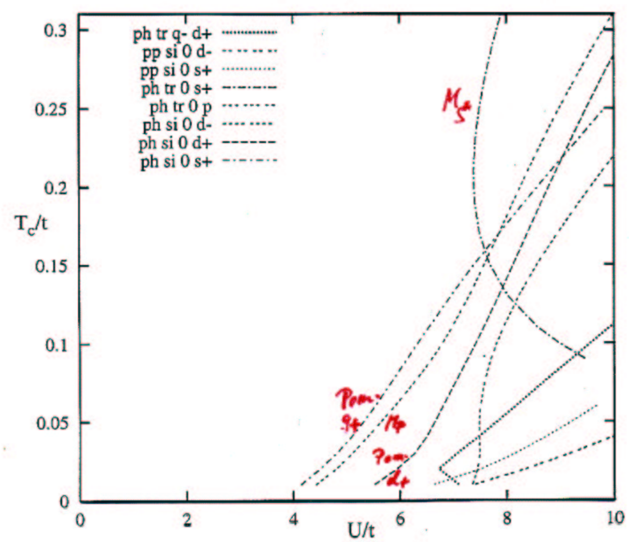
$t'/t = -1/6, \quad n = 0.86, \quad \mu/t = -0.667...0.659.$



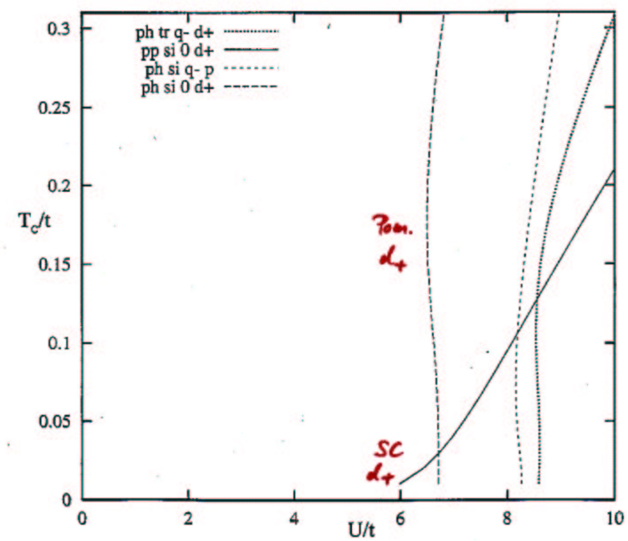
$t'/t = -1/3, \quad n = 0.68, \quad \mu/t = -1.339 \ldots -1.317$



$t'/t = -5/12, \quad n = 0.40, \quad \mu/t = -1.822 \ldots -1.877.$



$t'/t = -5/12, \quad n = 0.53, \quad \mu/t = -1.682\ldots - 1.665.$



$t'/t = -5/12, \quad n = 0.90, \quad \mu/t = -1.109\ldots - 0.985.$

Conclusion

The Hubbard-model shows surprisingly many possibilities of orderings at low temperatures.
Future goals: Investigation of the behavior in the symmetry broken phases.
A systematic integration with respect to the flow-parameter l.