Phase transitions in Hubbard Model
Anti-ferromagnetic and superconducting order in the Hubbard model

A functional renormalization group study

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Phase diagram
Mermin-Wagner theorem?

No spontaneous symmetry breaking of continuous symmetry in $d=2$!

not valid in practice!
Phase diagram
Goldstone boson fluctuations

- spin waves (anti-ferromagnetism)
- electron pairs (superconductivity)
Flow equation for average potential

\[ \partial_k U_k(\varphi) = \frac{1}{2} \sum_i \int \frac{d^d q}{(2\pi)^d} \frac{\partial_k R_k(q^2)}{Z_k q^2 + R_k(q^2) + \bar{M}_{k,i}^2(\varphi)} \]

\[ \bar{M}_{k,ab}^2 = \frac{\partial^2 U_k}{\partial \varphi_a \partial \varphi_b} : \text{ Mass matrix} \]

\[ \bar{M}_{k,i}^2 : \text{ Eigenvalues of mass matrix} \]
Simple one loop structure – nevertheless (almost) exact
Scaling form of evolution equation

\[ u = \frac{U_k}{k^d} \]
\[ \tilde{\rho} = Z_k k^{2-d} \rho \]
\[ u' = \frac{\partial u}{\partial \tilde{\rho}} \text{ etc.} \]

On r.h.s.: neither the scale k nor the wave function renormalization Z appear explicitly.

Scaling solution: no dependence on t; corresponds to second order phase transition.
Solution of partial differential equation:

yields highly nontrivial non-perturbative results despite the one loop structure!

Example:
Kosterlitz-Thouless phase transition
Anti-ferromagnetism in Hubbard model

- SO(3) – symmetric scalar model coupled to fermions
- For low enough k: fermion degrees of freedom decouple effectively
- Crucial question: running of $\kappa$ (location of minimum of effective potential, renormalized, dimensionless)
Critical temperature

For $T < T_c$: $\kappa$ remains positive for $k/t > 10^{-9}$

size of probe $> 1$ cm

$T/t = 0.05$

$T/t = 0.1$

$T_c = 0.115$

local disorder
pseudo gap
SSB

$\kappa_a = \frac{Z_a t^2}{T} \alpha_0$
Below the pseudocritical temperature

the reign of the goldstone bosons

effective nonlinear $O(3) - \sigma$ - model
critical behavior

for interval $T_c < T < T_{pc}$
evolution as for classical Heisenberg model
cf. Chakravarty, Halperin, Nelson
critical correlation length

\[ \xi_t = c(T) \exp \left\{ 20.7 \beta(T) \frac{T_c}{T} \right\} \]

c, \beta : slowly varying functions

exponential growth of correlation length
compatible with observation!

at \( T_c \) : correlation length reaches sample size!
Mermin-Wagner theorem?

No spontaneous symmetry breaking of continuous symmetry in $d=2$!

not valid in practice!
Below the critical temperature:

Infinite-volume-correlation-length becomes larger than sample size.

Finite sample \(\approx\) finite \(k\) : order remains effectively.

\[ T_{c}/t = 0.115 \]

Temperature in units of \( t \)

Antiferromagnetic order parameter
Action for Hubbard model

\[ S = \sum_{Q} \hat{\psi}^\dagger(Q) \left[ i\omega_{Q} + \xi_{Q} \right] \hat{\psi}(Q) \]

\[ + \frac{U}{2} \sum_{K_{1}, K_{2}, K_{3}, K_{4}} \left[ \hat{\psi}^\dagger(K_{1}) \hat{\psi}(K_{2}) \right] \left[ \hat{\psi}^\dagger(K_{3}) \hat{\psi}(K_{4}) \right] \delta(K_{1} - K_{2} + K_{3} - K_{4}). \]

\[ \hat{\psi}(Q) = \left( \hat{\psi}_{\uparrow}(Q), \hat{\psi}_{\downarrow}(Q) \right)^{T} \]

\[ \xi(q) = -\mu - 2t(\cos q_{x} + \cos q_{y}) - 4t' \cos q_{x} \cos q_{y} \]

\[ \sum_{Q} = T \sum_{n=-\infty}^{\infty} \int_{-\pi}^{\pi} \frac{d^{2}q}{(2\pi)^{2}}, \]

\[ \delta(Q - Q') = T^{-1} \delta_{n,n'} (2\pi)^{2} \delta(2)(q - q') \]
Truncation for flowing action

\[ \Gamma_k[\chi] = \Gamma_{F,k} + \Gamma_{Fm,k} + \Gamma_{F\rho,k} + \Gamma_{Fs,k} + \Gamma_{Fd,k} + \Gamma_{a,k} + \Gamma_{\rho,k} + \Gamma_{s,k} + \Gamma_{d,k} + \sum_X U_{B,k}(a, \rho, s, d) \]

\[ \Gamma_F = \Gamma_{F\text{kin}} + \Gamma^U_F \]

\[ \Gamma_{F\text{kin}} = \sum_Q \psi^\dagger(Q) P_F(Q) \psi(Q) \]

\[ P_F(Q) = Z_F(\omega_Q) (i\omega_Q + \xi(q)) \]

\[ \Gamma^U_F = \frac{1}{2} \sum_{K_1, K_2, K_3, K_4} U \delta(K_1 - K_2 + K_3 - K_4) \times [\psi^\dagger(K_1) \psi(K_2)] [\psi^\dagger(K_3) \psi(K_4)] . \]
Additional bosonic fields

- anti-ferromagnetic
- charge density wave
- s-wave superconducting
- d-wave superconducting

Initial values for flow: bosons are decoupled auxiliary fields (microscopic action)
Effective potential for bosons

\[
\sum \mathcal{U}_B(a, \rho, s, d) = \sum \frac{1}{2} \left( \tilde{m}_a^2 a^T (-Q)a(Q) + \tilde{m}_\rho^2 \rho(-Q)\rho(Q) \right) \\
+ \tilde{m}_s^2 s^*(Q)s(Q) + \tilde{m}_d^2 d^*(Q)d(Q) \\
+ \frac{1}{2} \sum_{Q_1, Q_2, Q_3, Q_4} \delta(Q_1 + Q_2 + Q_3 + Q_4) \\
\times \left( \tilde{\lambda}_a \alpha(Q_1, Q_2)\alpha(Q_3, Q_4) \\
+ \lambda_d \delta(Q_1, Q_2)\delta(Q_3, Q_4) \\
+ 2\lambda_{ad} \alpha(Q_1, Q_2)\delta(Q_3, Q_4) \right),
\]

\[
\sum \mathcal{U}_B(a, d) = \frac{1}{2} \sum_{Q_1, Q_2, Q_3, Q_4} \delta(Q_1 + Q_2 + Q_3 + Q_4) \\
\times \left( \tilde{\lambda}_a \left[ \alpha(Q_1, Q_2) - \alpha_0\delta(Q_1)\delta(Q_2) \right] \\
\times \left[ \alpha(Q_3, Q_4) - \alpha_0\delta(Q_3)\delta(Q_4) \right] \\
+ \lambda_d \left[ \delta(Q_1, Q_2) - \delta_0\delta(Q_1)\delta(Q_2) \right] \\
\times \left[ \delta(Q_3, Q_4) - \delta_0\delta(Q_3)\delta(Q_4) \right] \\
+ 2\lambda_{ad} \left[ \alpha(Q_1, Q_2) - \alpha_0\delta(Q_1)\delta(Q_2) \right] \\
\times \left[ \delta(Q_3, Q_4) - \delta_0\delta(Q_3)\delta(Q_4) \right] \right),
\]

SYM

microscopic: only “mass terms”

SSB
Yukawa coupling between fermions and bosons

\[ \Gamma_{Fa} = - \sum_{K, Q, Q'} \vec{h}_a(K) \cdot [\psi^*(Q) \sigma \psi(Q')] \delta(K - Q + Q' + \Pi), \]

\[ \Gamma_{Fp} = - \sum_{K, Q, Q'} \vec{h}_p(K) \rho(K) [\psi^*(Q) \psi(Q')] \delta(K - Q + Q'), \]

\[ \Gamma_{Fs} = - \sum_{K, Q, Q'} \vec{h}_s(K) \left( s^*(K) [\psi^T(Q) \epsilon \psi(Q')] \right) \delta(K - Q - Q'), \]

\[ \Gamma_{Fd} = - \sum_{K, Q, Q} \vec{h}_d(K) f_d ((Q - Q')/2) \left( d^*(K) [\psi^T(Q) \epsilon \psi(Q')] \right) \delta(K - Q - Q'), \]

\[ f_d(Q) = f_d(q) = \frac{1}{2} \left( \cos(q_x) - \cos(q_y) \right) \]

Microscopic Yukawa couplings vanish!
Kinetic terms for bosonic fields

\[ \Gamma_a = \frac{1}{2} \sum_Q a^T(-Q) P_a(Q) a(Q), \]
\[ \Gamma_\rho = \frac{1}{2} \sum_Q \rho(-Q) P_\rho(Q) \rho(Q), \]
\[ \Gamma_s = \sum_Q s^*(Q) P_s(Q) s(Q), \]
\[ \Gamma_d = \sum_Q d^*(Q) P_d(Q) d(Q). \]

anti-ferromagnetic boson

d-wave superconducting boson

\[ a(Q) = m(Q + \Pi) \]
incommensurate anti-ferromagnetism

\[ P_a(Q) = Z_a \omega_Q^2 + A_a F(q) \]

commensurate regime:

\[ F_c(q) = \frac{D_a^2 \cdot [q]^2}{D_a^2 + [q]^2} \]

\[ [q]^2 = q_x^2 + q_y^2 \text{ for } q_{x,y} \in [-\pi, \pi] \]

incommensurate regime:

\[ F_i(q, \hat{q}) = \frac{D_a^2 \tilde{F}(q, \hat{q})}{D_a^2 + \tilde{F}(q, \hat{q})} \]

\[ \tilde{F}(q, \hat{q}) = \frac{1}{4\hat{q}^2}((\hat{q}^2 - [q]^2)^2 + 4[q_x]^2[q_y]^2) \]

\[ D_a = \frac{1}{A_a} (\hat{P}_a(0, \pi, \pi) - \hat{P}_a(0, \hat{q}, 0)) \]
infrared cutoff

\[ R_k^F (Q) = \text{sgn}(\xi(q)) (k - |\xi(q)|) \Theta(k - |\xi(q)|) \]

\[ R_k^{a/\rho} (Q) = A_{a/\rho} \cdot \left(\frac{k^2}{t^2} - F_{c/i}(q, \hat{q})\right) \Theta\left(\frac{k^2}{t^2} - F_{c/i}(q, \hat{q})\right) \]

linear cutoff (Litim)
flowing bosonisation

effective four-fermion coupling in appropriate channel

is translated to bosonic interaction at every scale $k$

H.Gies, ...

\[
\Gamma_k[\psi, \psi^*, \phi] = \sum_Q \psi^*(Q) P_{\psi,k} \psi(Q) + \frac{1}{2} \sum_Q \phi(-Q) P_{\phi,k}(Q) \phi(Q) - \sum_Q h_k(Q) \phi(Q) \bar{\phi}(-Q) + \sum_Q \lambda_{\psi,k}(Q) \bar{\phi}(Q) \bar{\phi}(-Q)
\]

k-dependent field redefinition

\[
\phi_k(Q) = \phi_{\bar{k}}(Q) + \Delta \alpha_k(Q) \bar{\phi}(Q)
\]

\[
\partial_k \phi_k(Q) = - \partial_k \alpha_k(Q) \bar{\phi}(Q)
\]

absorbs four-fermion coupling
running Yukawa couplings
flowing boson mass terms

SYM: close to phase transition
Pseudo-critical temperature $T_{pc}$

Limiting temperature at which bosonic mass term vanishes ($\kappa$ becomes nonvanishing)

It corresponds to a diverging four-fermion coupling

This is the “critical temperature” computed in MFT!

Pseudo-gap behavior below this temperature
Pseudocritical temperature

\[ T_{pc} \]

\[ T_c \]

Flow eq.

MFT(HF)

\[ \mu \]
Critical temperature

For $T < T_c$: $\kappa$ remains positive for $k/t > 10^{-9}$
size of probe > 1 cm

$T/t = 0.05$

$T/t = 0.1$

local disorder
pseudo gap

SSB

$\kappa_a = \frac{Z_a t^2}{T} \alpha_0$

$T_c = 0.115$
Phase diagram

Pseudo-critical temperature
spontaneous symmetry breaking of
abelian continuous symmetry in $d=2$

Bose –Einstein condensate

Superconductivity in
Hubbard model

Kosterlitz – Thouless
phase transition
Essential scaling: \( d=2, N=2 \)

- Flow equation contains correctly the non-perturbative information!
- (essential scaling usually described by vortices)

\[ m_R \sim \exp \left\{ - \frac{b}{(T-T_c)^{1/2}} \right\}, T > T_c \]

\[ \kappa_\lambda \sim (T_c - T) + \text{const} \]

Von Gersdorff …
Kosterlitz-Thouless phase transition
(d=2, N=2)

Correct description of phase with
Goldstone boson
(infinite correlation length)
for $T < T_c$
Temperature dependent anomalous dimension $\eta$
Running renormalized d-wave superconducting order parameter $\kappa$ in doped Hubbard (-type) model

$\kappa \sim -\ln \left(\frac{k}{\Lambda}\right)$

$T > T_c$  $T < T_c$

C. Krahl, …

location of minimum of $u$

local disorder pseudo gap

macroscopic scale 1 cm
Renormalized order parameter $\kappa$ and gap in electron propagator $\Delta$ in doped Hubbard-type model
order parameters in Hubbard model
Competing orders
Anti-ferromagnetism suppresses superconductivity
coexistence of different orders?
quartic couplings for bosons
conclusions

- functional renormalization gives access to low temperature phases of Hubbard model
- order parameters can be computed as function of temperature and chemical potential
- competing orders
- further quantitative progress possible
changing degrees of freedom
flowing bosonisation

- adapt bosonisation to every scale $k$ such that

is translated to bosonic interaction

H.Gies, ...

\[ \Gamma_k[\psi, \psi^*, \phi] = \sum_Q \psi^*(Q) P_{\psi,k} \psi(Q) + \frac{1}{2} \sum_Q \phi(-Q) P_{\phi,k}(Q) \phi(Q) - \sum_Q h_k(Q) \phi(Q) \phi(-Q) + \sum_Q \lambda_{\psi,k}(Q) \phi(Q) \phi(-Q) \]

k-dependent field redefinition

\[ \phi_k(Q) = \phi_{\bar{k}}(Q) + \Delta \alpha_k(Q) \tilde{\phi}(Q) \]

\[ \partial_k \phi_k(Q) = - \partial_k \alpha_k(Q) \tilde{\phi}(Q) \]

absorbs four-fermion coupling
flowing bosonisation

Evolution with $k$-dependent field variables

Modified flow of couplings

Choose $\alpha_k$ in order to absorb the four fermion coupling in corresponding channel

\[
\begin{align*}
\partial_k h_k(Q) &= \partial_k h_k(Q)|_{\phi_k} + \partial_k \alpha_k(Q) P_{\phi, k}(Q), \\
\partial_k \lambda_{\psi, k}(Q) &= \partial_k \lambda_{\psi, k}(Q)|_{\phi_k} + h_k(Q) \partial_k \alpha_k(Q).
\end{align*}
\]

\[
\begin{align*}
\partial_k h_k(Q) &= \partial_k h_k(Q)|_{\phi_k} - \frac{P_{\phi, k}(Q)}{h_k(Q)} \partial_k \lambda_{\psi, k}(Q)|_{\phi_k}
\end{align*}
\]
Mean Field Theory (MFT)

Evaluate Gaussian fermionic integral in background of bosonic field, e.g.

\[ \hat{\rho}(Q) \to \rho \delta(Q) \]
\[ \hat{m}(Q) \to \bar{a} \delta(Q - \Pi) \]

\[ Z_{\text{MF}} = \int \mathcal{D}(\hat{\psi}^*, \hat{\psi}) \exp(-S_{\text{MF}}), \]
\[ S_{\text{MF}} = \sum_Q \hat{\psi}^\dagger(Q)(i \omega_F - \mu - 2t(\cos q_1 + \cos q_2))\hat{\psi}(Q) \]
\[ - \sum_Q (U_\rho \rho \hat{\psi}^\dagger(Q)\hat{\psi}(Q) + U_m \bar{a} \hat{\psi}^\dagger(Q + \Pi)\bar{\sigma}\hat{\psi}(Q)) \]
\[ + \frac{V_2}{2T}(U_\rho \rho^2 + U_m \bar{a}^2) - J_\rho(0)\rho - J_m(-\Pi)\bar{a} \]

\[ U = -U_\rho + 3U_m \]

\[ \Gamma_{\text{MF}} = -\ln Z_{\text{MF}} + J_\rho(0)\rho + J_m(-\Pi)\bar{a} \]
Mean field phase diagram

for two different choices of couplings – same U!
Mean field ambiguity

$T_c$

$U_m = U_q = U/2$

$U_m = U/3 , U_q = 0$

Artefact of approximation …

cured by inclusion of bosonic fluctuations

J.Jaeckel,…

Mean field phase diagram

$U = -U_\rho + 3U_m$
Bosonisation and the mean field ambiguity
Bosonic fluctuations

fermion loops

boson loops

mean field theory
Bosonisation cures mean field ambiguity

\[ T_c \]

\[ \frac{U_q}{t} \]

\[ \rho \]

\[ U \]

HF/SD

MFT

Flow eq.

\[
\begin{align*}
T & \quad 3.8 \\
& \quad 3.6 \\
& \quad 3.4 \\
& \quad 3.2 \\
& \quad 3.0 \\
& \quad 2.8 \\
& \quad 2.6 \\
& \quad 2.4 \\
& \quad 2.2 \\
& \quad 2.0 \\
\end{align*}
\]

\[
\begin{align*}
U_q/t & \quad 1.8 \\
& \quad 2.0 \\
& \quad 2.2 \\
& \quad 2.4 \\
& \quad 2.6 \\
& \quad 2.8 \\
& \quad 3.0 \\
& \quad 3.2 \\
& \quad 3.4 \\
& \quad 3.6 \\
& \quad 3.8 \\
\end{align*}
\]
quartic couplings for bosons
kinetic and gradient terms for bosons
fermionic wave function renormalization