Self-energy Flow in the Hubbard Model

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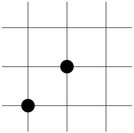
Outline of talk

RG study of Hubbard model: flow of interaction vertex and two point function

- Introduction
  - $2d$ Fermionic Hubbard model
  - Interaction vertex parametrisation and RG flows
- Self-energy flow
  - Parametrisation of self-energy: Hopping parameter corrections, Z factor
  - Extraction of information from flow equation
  - Feedback on interaction vertex flow
- Conclusions and future work

Hubbard Model

Spin $\frac{1}{2}$ fermions on torus $\Gamma = (\mathbb{Z}_L)^2$ of size L



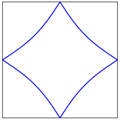
$$H = \sum_{\substack{\mathbf{x},\mathbf{y} \\ s}} a^+_{\mathbf{x},s} \; t(\mathbf{x}-\mathbf{y}) \; a_{\mathbf{y},s} + U \sum_{\mathbf{x}} n_{\mathbf{x},\uparrow} \; n_{\mathbf{x},\downarrow}, \qquad U > 0$$

Momentum space representation

$$H = \sum_{\mathbf{p},s} \varepsilon(\mathbf{p}) \; c^+_{\mathbf{p},s} c_{\mathbf{p},s} + \frac{U}{|\Gamma|} \sum_{\mathbf{k},\mathbf{p},\mathbf{q}} c^+_{\mathbf{p}+\mathbf{k},\downarrow} c^+_{\mathbf{q}-\mathbf{k},\uparrow} \; c_{\mathbf{q},\uparrow} c_{\mathbf{p},\downarrow}$$

Dispersion relation

$$\begin{aligned} \varepsilon(p_x, p_y) = & -2t_1 \; (\cos p_x + \cos p_y) \\ & + 4t_2 \; (\cos p_x \cos p_y + 1) - \mu \end{aligned}$$



(set $t_1 = 1$)

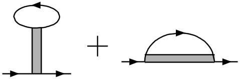
1PI one loop RG

- Partition function $Z_{\Omega}(h) = Z(Q_{\Omega}, V)(h)$
- Flow equation for 1PI generating functional $\Gamma_{\Omega}(\psi)$

$$\dot{\Gamma}_{\Omega}(\psi) = \mathrm{Tr}\ \dot{Q}_{\Omega}\ (\delta^2\Gamma_{\Omega})^{-1}(\psi), \qquad \Gamma_{\Omega_0}(\psi) = \Gamma^{(0)}(\psi)$$

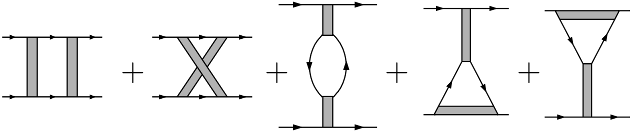
- formal power series expansion in field ψ
- 1 loop truncation for $U(1)$ and $SU(2)$ invariant vertex functions

$\dot{\Sigma}_{\Omega}(k) =$



$k = (k_0, \mathbf{k})$

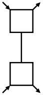
$\dot{v}_{\Omega}(k_1 \ldots k_4) =$

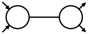


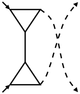
[Wetterich 1993; Salmhofer 1998; Honerkamp, Salmhofer 2001]

Vertex parametrisation via exchange bosons

- Vertex decomposition in 3 channels: scattering, superconducting and magnetic channels
- interacting charge/Cooper pair/spin operators with *specific transfer momenta*

$v_K(k_1 \dots k_4) =$  $= -\sum_{m,n} f_m(\mathbf{k}_1 + \frac{\mathbf{k}_2 - \mathbf{k}_3}{2})\, K_{mn}(k_2 - k_3)\, f_n(\mathbf{k}_2 - \frac{\mathbf{k}_2 - \mathbf{k}_3}{2})$

$v_{SC}(k_1 \dots k_4) =$  $= -\sum_{m,n} f_m(\frac{\mathbf{k}_1 + \mathbf{k}_2}{2} - \mathbf{k}_1)\, D_{mn}(k_1 + k_2)\, f_n(\frac{\mathbf{k}_1 + \mathbf{k}_2}{2} - \mathbf{k}_3)$

$v_M(k_1 \dots k_4) =$  $= +\sum_{m,n} f_m(\mathbf{k}_1 - \frac{\mathbf{k}_1 - \mathbf{k}_3}{2})\, M_{mn}(k_1 - k_3)\, f_n(\mathbf{k}_2 + \frac{\mathbf{k}_1 - \mathbf{k}_3}{2})$

- distribute vertex flow according to singular momentum structure to channels
- obtain flow equation for exchange propagators K, D, M

[Husemann, Salmhofer 2008]

Choice of Regulator function

- self-energy flow produces *Fermi surface flow*
- *momentum cutoff* around Fermi surface: would need adaptive scheme
- use *soft frequency regulator*: replace propagator

$$C = \frac{1}{i\omega - \varepsilon} \longrightarrow C_{\Omega} = \frac{1}{i\omega - \varepsilon}\, \chi_{\Omega}(\omega),$$

$$\chi_{\Omega}(\omega) = \frac{\omega^2}{\omega^2 + \Omega^2}, \quad \Omega > 0$$

- effective regularisation for $\Omega > 0$
- initial condition at scale $\Omega = \Omega_0 > 0$, Ω_0 large
- cannot enter symmetry broken regime: stop flow at critical scale $\Omega = \Omega_c, \quad 0 < \Omega_c < \Omega_0$
- no artificial suppression of small-momentum particle-hole processes

Self-energy zero-mode

- flowing Fermi surface results in *scale dependent particle density*
- one possible definition of particle density during flow:

  propagator of interacting system during flow is

$$
\begin{aligned}
G_\Omega(p) &= \left(C_\Omega^{-1} + \Sigma_\Omega\right)^{-1}(p), && p = (\omega, \mathbf{p}) \\
&= \frac{\chi_\Omega(\omega)}{i\omega - \varepsilon(\mathbf{p}) + \chi_\Omega(\omega)\ \Sigma_\Omega(p)}, && \chi_\Omega(\omega) = \frac{\omega^2}{\omega^2 + \Omega^2}
\end{aligned}
$$

  define particle density

$$
\varrho_\Omega := \int \mathrm{d}p\ G_\Omega(p)
$$

- adjust flow such that $\dot{\varrho}_\Omega = 0$
- choose ϱ_Ω to be van-Hove-filling of interacting system (at Ω_c)

Parametrisation of self-energy

- *large frequency* behaviour (read off flow equation)

$$\Sigma(\omega, \mathbf{p}) = cte. + \mathcal{O}(\frac{1}{\omega})$$

- *small frequency* dependence: we expect

$$\Sigma(\omega, \mathbf{p}) = \Sigma_0(\mathbf{p}) + i\omega\ \Sigma_1(\mathbf{p}) + \mathcal{O}(\omega^2 \ln^\alpha \omega)$$

- singularities of propagator play essential rôle, located at *small* frequencies (and momenta close to Fermi surface)
- capture well singularities in propagator of interacting system: *small frequency expansion as an ansatz for self-energy*, examine $\Sigma_0(\mathbf{p})$, $\Sigma_1(\mathbf{p})$
- in a first step: examine $\Sigma_0(\mathbf{p})$, $\Sigma_1(\mathbf{p})$ separately

Frequency independent self-energy: $\Sigma_0(\mathbf{p})$

- Ansatz: sum of corrections to hopping terms g_i (ONS)

$$\Sigma_0(\mathbf{p}) = \sum_{i=0}^{n} \delta t_i \; g_i(\mathbf{p})$$

- Extraction of $\delta \dot{t}_i$ from flow equation:

Fourier analysis vs. *Differentiation*

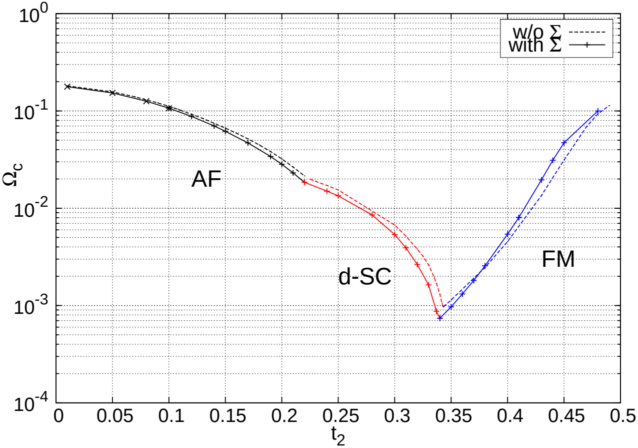
$$\delta \dot{t}_i = \left\langle g_i, \dot{\Sigma}_0 \right\rangle, \qquad i = 1 \dots n$$

vs.

$$\left(D_j \; \dot{\Sigma}_0 \right)(\mathbf{p}_j) = \mathbf{a}^{(j)} \cdot \delta \dot{\mathbf{t}}, \qquad j = 1 \dots n$$

- Results compare well if $\{\mathbf{p}_j\}$ are not chosen in a small region of the Brillouin zone, only

Feedback of Σ_0 on interaction vertex ($U = 3$, $T = 0$)



- small changes in critical scale
- location of ordering tendencies almost unchanged

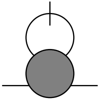
Frequency dependent self-energy: $\Sigma_1(\mathbf{p})$ ($T = 0$)

- Small frequency behaviour of self-energy: study Z factor

$$Z_\Omega(\mathbf{p}) = 1 + \frac{1}{i}(\partial_{p_0}\ \Sigma)(p_0 = 0, \mathbf{p})$$

- start by neglecting frequency-independent self-energy
- Flow equation:

$$\dot{Z}_\Omega(\mathbf{p}) = \frac{1}{i}\partial_{p_0}$$



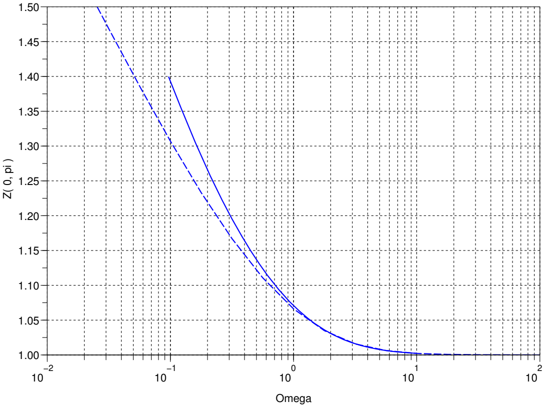
(p)

- frequency dependence of interaction vertex is important
- here: discretisation of this frequency dependence rather than some standard ansatz

Flow of Z factor ($t_2 = 0.1, U = 3$)

Scale dependence of $Z(0, \pi)$
(curved Fermi surface and present van-Hove-singularity)

- perturbation theory: $Z_\Omega^{(2)}(0, \pi) \sim |\ln \Omega|$
- RG flow: enhancement of divergence

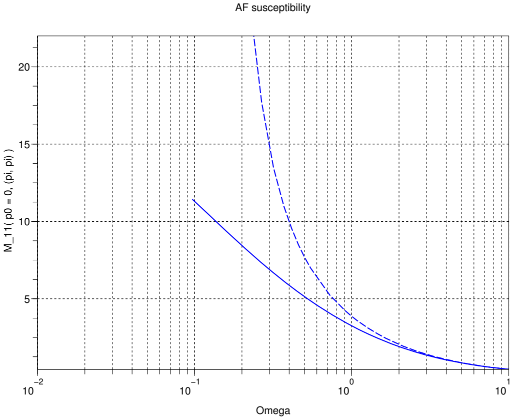


Dashed line: $Z^{(2)}(0, \pi)$, Solid line: $Z(0, \pi)$

Feedback Z factor on interaction vertex ($t_2 = 0.1, U = 3$)

AF susceptibility in parameter region of dominant AFM

- AFM remains dominant instability
- critical scale is significantly suppressed



Flow with (solid) and without (dashed) Z factor

- verify if strong suppression of critical scale is inherent property or artefact of small frequency expansion

Conclusions

- RG study of Hubbard model: trace flow of interaction vertex and two point function
- singular structure of propagator: especially examine small frequency behaviour of two point function

- frequency-independent self-energy: minor feedback on interaction vertex flow
- in progress: RG flow with frequency-dependent self-energy

Frequency independent self-energy: $\Sigma_0(\mathbf{p})$

- ansatz for $\Sigma_0(\mathbf{p})$: sum of corrections to hopping terms

$$\Sigma_0(\mathbf{p}) = \sum_{i=0}^{n} \delta t_i \; g_i(\mathbf{p})$$

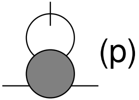
- conveniently choose $\{g_i\}$ as ONS,
  first elements $\mathbf{p} = (x, y)$

$$\begin{aligned} g_0(x,y) &= 1 \\ g_1(x,y) &= \cos x + \cos y \\ g_2(x,y) &= 2\cos x \cos y \\ g_3(x,y) &= \cos 2x + \cos 2y \\ &\dots \end{aligned}$$

Extracting information from flow equation

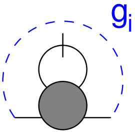
Several possibilities for extracting hopping corrections $\dot{\delta t}_i$ out of flow

$$\dot{\Sigma}_0(\mathbf{p}) = \sum_{i=0}^{n} \dot{\delta t}_i \; g_i(\mathbf{p})$$



- Global determination (Fourier analysis)

$$\dot{\delta t}_i = \left\langle g_i, \dot{\Sigma}_0 \right\rangle$$



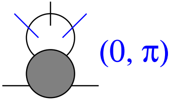
- Local determination

$$\left((-\partial_x^2 + \partial_y^2) \; \dot{\Sigma}_0 \right)(0,\pi) = \mathbf{a}^{(1)} \cdot \dot{\delta}\mathbf{t}$$

$$\left((\partial_x^2 + \partial_y^2) \; \dot{\Sigma}_0 \right)(0,\pi) = \mathbf{a}^{(2)} \cdot \dot{\delta}\mathbf{t}$$

$$\dot{\Sigma}_0(0,0) - \dot{\Sigma}_0(0,\pi) = \mathbf{a}^{(3)} \cdot \dot{\delta}\mathbf{t}$$

$$\dot{\Sigma}_0(\pi,\pi) - \dot{\Sigma}_0(0,\pi) = \mathbf{a}^{(4)} \cdot \dot{\delta}\mathbf{t}$$



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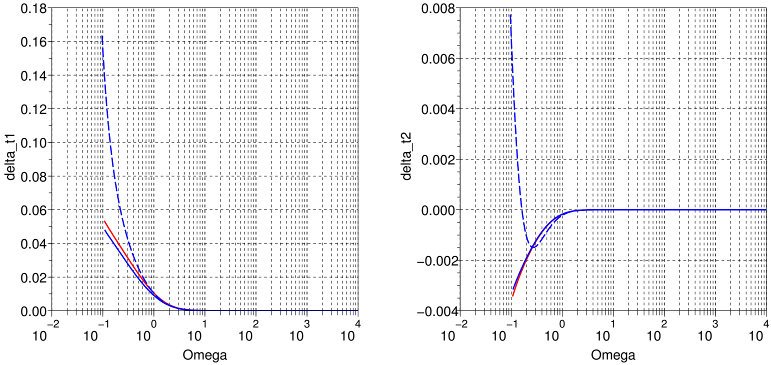
Compare extraction methods ($U = 3$, $t_2 = 0.1$)

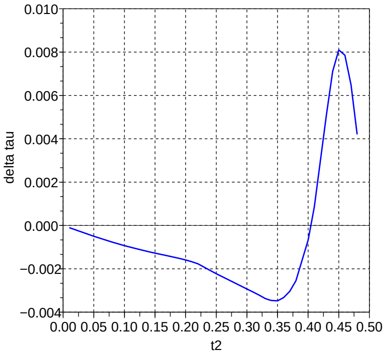


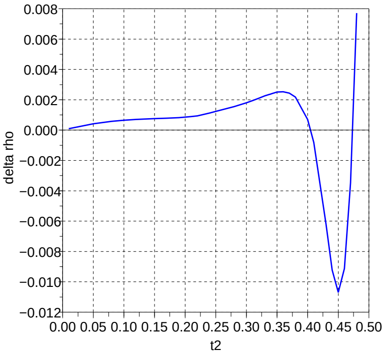
red: Fourier projection, blue: local examination

- results compare well if $\mathbf{a}^{(3)}, \mathbf{a}^{(4)}$ are included
- similar results in other parameter ranges, bigger discrepance in d-SC/FM transition region

Results: Fermi surface shift ($U = 3$, $T = 0$)

Interacting vs. non-interacting system at van Hove filling:





Ratio of hopping parameters

$$\delta\tau = \frac{t_2^{int}}{t_1^{int}} - \frac{t_2}{t_1}$$

Level shift

$$\delta\varrho = \varrho_{int} - \varrho_{free}$$

Matsubara summation

- evaluation of rhs of flow equations: compute Matsubara sums of propagators
- perform Matsubara sums by residues
- propagator of interacting system during flow

$$G_{\Omega}(p) = \left(C_{\Omega}^{-1} + \Sigma_{\Omega}\right)^{-1}(p), \qquad p = (\omega, \mathbf{p})$$
$$= \frac{\omega^2}{(i\omega - \varepsilon(\mathbf{p}))\ (\omega^2 + \Omega^2) + \omega^2\ \Sigma_{\Omega}(p)}$$

  involves polynomial of 3^{rd} degree in ω

- intricate dependence of location of pôles on parameters
- intricate dependence of summation result on parameters (unlike $\Sigma \equiv 0$)

Flow equations

$$\dot{D}_{mm}(l) = +\frac{1}{2}\int \mathrm{d}p\ L(-p, l+p)\ \mathcal{F}_m^2(-D, \frac{3M-K}{2})(p,l), \quad (m=1,2)$$
$$\dot{M}_{mm}(l) = -\frac{1}{2}\int \mathrm{d}p\ L(p, l+p)\ \mathcal{F}_m^2(M, \frac{-2D+M-K}{2})(p,l)$$
$$\dot{K}_{mm}(l) = -\frac{1}{2}\int \mathrm{d}p\ L(p, l+p)\ \mathcal{F}_m^2(-K, \frac{-2D+3M+K}{2})(p,l)$$

where

$L(p_1, p_2) = \partial_\Omega\ (\ G(p_1)G(p_2)\ )$
$s(p)$ single scale propagator,
$\mathcal{F}_m$ convolution with form factors

$f_1(x,y) = 1,\ f_2(x,y) = \cos x - \cos y$

Flow equations II

$$
\begin{aligned}
\mathcal{F}_1(A,B)(p,l) =& U + A_{11}(l) + \int \text{đ}\mathbf{u}\ B_{11}(\frac{l_0}{2} + p_0, \mathbf{u}) \\
&+ \int \text{đ}\mathbf{u}\ B_{22}(\frac{l_0}{2} + p_0, \mathbf{u})\ f_2(\mathbf{p} - \frac{\mathbf{u}}{2})\ f_2(\mathbf{p} + \mathbf{l} - \frac{\mathbf{u}}{2}) \\
\mathcal{F}_2(A,B)(p,l) =& A_{22}(l)\ f_2(\mathbf{p} + \frac{\mathbf{l}}{2}) \\
&+ \int \text{đ}\mathbf{u}\ f_2(\mathbf{p} + \frac{\mathbf{l}}{2} - \mathbf{u})\ \Big(B_{11}(\frac{l_0}{2} + p_0, \mathbf{u}) \\
&\quad + B_{22}(\frac{l_0}{2} + p_0, \mathbf{u})\ f_2(\mathbf{p} - \frac{\mathbf{u}}{2})\ f_2(\mathbf{p} + \mathbf{l} - \frac{\mathbf{u}}{2}) \Big)
\end{aligned}
$$

form factors: $f_1(x,y) = 1,\ f_2(x,y) = \cos x - \cos y$

Flow equations III

$$
\begin{aligned}
\dot{\Sigma}(k) =& \frac{1}{2}(-U + K_{11}(0)) \int \mathrm{d}p\; s(p) \\
& + \frac{1}{2} \int \mathrm{d}p\; s(p-k)\; \Big(D_{11}(p) + D_{22}(p)\; f_2^2(\frac{\mathbf{p}}{2} - \mathbf{k}) \Big) \\
& - \frac{1}{2^2} \int \mathrm{d}p\; s(p+k)\; \left(K_{11}(p) + 3 M_{11}(p) \right) \\
\dot{\varrho} =& 0
\end{aligned}
$$

Perturbation theory: Bubble frequency dependence

Particle-hole bubble $\mathcal{B}^+(l) = U^2 \int \mathrm{d}p \; C_\Omega(p) C_\Omega(l+p), \quad l = (l_0, \mathbf{l})$

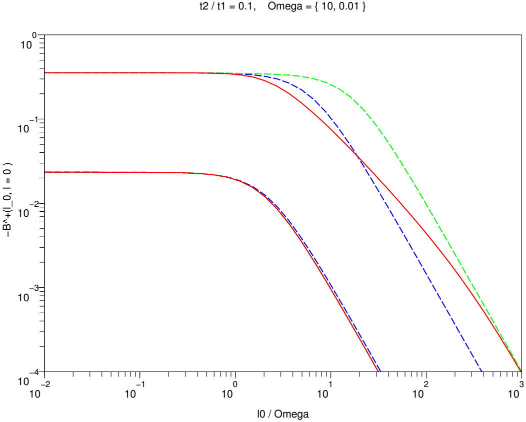
$\varepsilon(-\mathbf{p}) = \varepsilon(\mathbf{p}) \implies \mathcal{B}^+(l) \in \mathbb{R} \; \forall l$

Parametrisations:

$$\mathcal{B}_1^+(l) = \frac{1}{m_\mathbf{l}^2 + b_\mathbf{l}^2 \; l_0^2}$$

$$\mathcal{B}_2^+(l) = \frac{1}{m_\mathbf{l}^2 + b_\mathbf{l}^2 \; l_0^2} \frac{c_\mathbf{l}^2 + l_0^2}{d_\mathbf{l}^2 + l_0^2}$$

red $\mathcal{B}^+$, blue $\mathcal{B}_1^+$, green $\mathcal{B}_2^+$



Existence of independent intermediate frequency regime