Quantum Criticality in fRG+MF

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This work continues previous fRG studies of the two-dimensional repulsive Hubbard model by Giering, Husemann and Salmhofer.[1,2,3]

[1] Kay-Uwe Giering and Manfred Salmhofer. In: *Phys. Rev. B* 86 (24 Dec. 2012).

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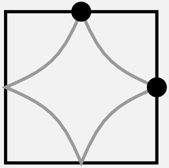
Hubbard model:

$$H = \sum_{\sigma \in \{+,-\}} \sum_{\boldsymbol{p} \in \mathbb{L}^*} \big(\epsilon(\boldsymbol{p}) - \mu\big) c_\sigma^+(\boldsymbol{p}) c_\sigma(\boldsymbol{p}) + \frac{U}{L^2} \sum_{\boldsymbol{p},\boldsymbol{q},\boldsymbol{\ell} \in \mathbb{L}^*} c_+^+(\boldsymbol{p}+\boldsymbol{\ell}) c_-^+(\boldsymbol{q}-\boldsymbol{\ell}) c_-(\boldsymbol{q}) c_+(\boldsymbol{p})$$



$$\epsilon\big(\boldsymbol{k} = (x,y)\big) = -2t\big(\cos x + \cos y\big) + 4t'\big(\cos x \cos y + 1\big)$$

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> fRG flow in Katanin's scheme
> with momentum and frequency dependent vertex
> and purely imaginary frequency dependent self-energy

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Main Result:

> Evidence of a QCP
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> at van Hove filling and in the vicinity of $t'/t = 0.341$

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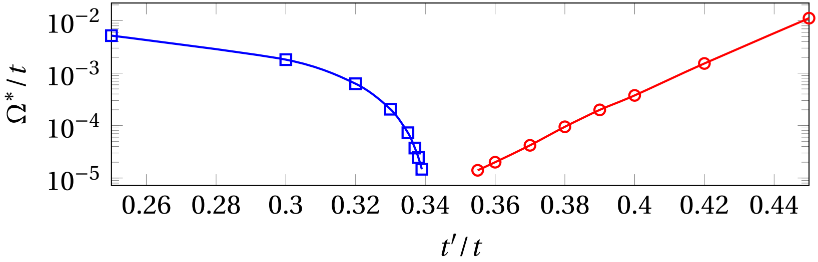

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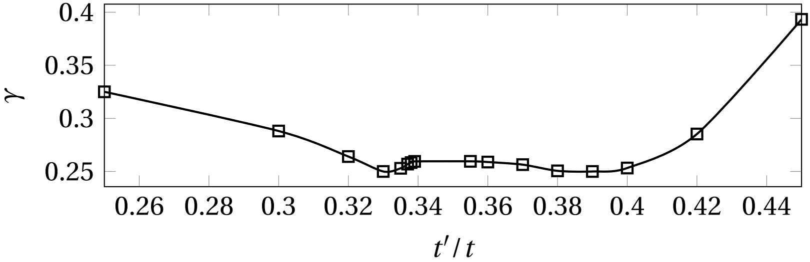

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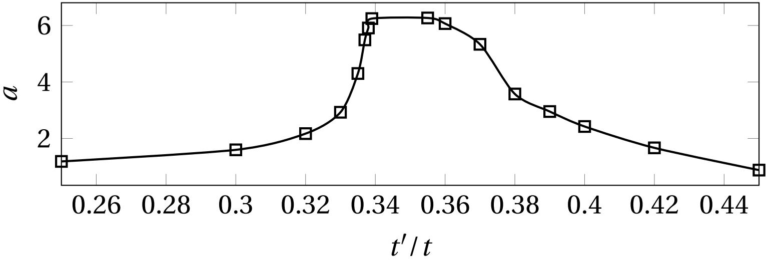

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Consider the IR regular propagator

$$c_\Omega(p) = \frac{\chi_\Omega(p_p)}{\mathrm{i}\, p_0 - \xi(\boldsymbol{p})} \quad , \quad \chi_\Omega(p_0) = \frac{p_0^2}{p_0^2 + \Omega^2}$$

The partition function is given by

$$\begin{aligned} Z = \int \mathrm{d}\mu_C(\psi,\overline{\psi})\, \mathrm{e}^{V(\psi,\overline{\psi})} &= \int \mathrm{d}\mu_{C-C_\Omega}(\psi,\overline{\psi}) \int \mathrm{d}\mu_{C_\Omega}(\eta,\overline{\eta})\, \mathrm{e}^{V(\psi+\eta,\overline{\psi}+\overline{\eta})} \\ &= \int \mathrm{d}\mu_{C-C_\Omega}(\psi,\overline{\psi})\, \mathrm{e}^{-\mathscr{A}_\Omega(\psi,\overline{\psi})} \end{aligned}$$

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$$= \int \mathrm{d}\mu_{C-C_\Omega}(\psi, \overline{\psi})\, \mathrm{e}^{-\mathscr{A}_\Omega(\psi,\overline{\psi})}$$

where $\mathscr{A}_\Omega$ is the generator of the amputated connected green functions.

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where $\mathscr{A}_\Omega$ is the generator of the amputated connected green functions.

$$A_\Omega^{(2)} = -C_\Omega^{-1} + C_\Omega^{-1} G_\Omega C_\Omega^{-1} = \Sigma_\Omega + \Sigma_\Omega C_\Omega \Sigma_\Omega + \Sigma_\Omega C_\Omega \Sigma_\Omega C_\Omega \Sigma_\Omega + \cdots$$

$$A_\Omega^{(4)}(\sigma_1 k_1, \ldots, \sigma_4 k_4) = \Gamma_\Omega^{(4)}(\sigma_1 k_1, \ldots, \sigma_4 k_4) \prod_{i=1}^{4} \frac{G_\Omega(k^{(i)})}{C_\Omega(k^{(i)})}$$

Identify relevant interaction in each channel

$$\mathrm{FM}: Z = \int \mathrm{d}\mu_T(\Psi, \overline{\Psi})\, \mathrm{e}^{\frac{1}{4\beta \mathrm{V}} M_{1,1}(0) S^{(3)}(0) S^{(3)}(0) + \cdots}$$

$$\mathrm{dSC}: Z = \int \mathrm{d}\mu_T(\Psi, \overline{\Psi})\, \mathrm{e}^{-\frac{1}{\beta \mathrm{V}} D_{2,2}(0) \bar{C}_2^{(2)}(0) C_2^{(2)}(0) + \cdots}$$

$S^j_\ell, C^j_\ell, \bar{C}^j_\ell$ stand for the fermionic bilinears

$$S^{(j)}(\ell) = \int_q \bar{\psi}_q \sigma^{(j)} \psi_{q+\ell}$$

$$\bar{C}^{(j)}_m(\ell) = \frac{\mathrm{i}}{2} \int_q \bar{\psi}_q \sigma^{(j)} \bar{\psi}_{\ell - q}$$

$$C^{(j)}_m(\ell) = \frac{\mathrm{i}}{2} \int_q f_m(\boldsymbol{q}) \psi_q \sigma^{(j)} \psi_{\ell - q}$$

where

$$f_1(\boldsymbol{k}) = 1 \quad , \quad f_2(\boldsymbol{k}) = \cos(k_x) - \cos\left(k_y\right)$$

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Hubbard-Stratonovich transformation:

$$\mathrm{e}^{a^2/4} = \frac{1}{\sqrt{\pi}} \int_{\mathbb{R}} \mathrm{e}^{-\phi^2 + \phi a}\, \mathrm{d}\phi$$

$$\mathrm{e}^{ab} = \int_{\mathbb{C}} \mathrm{e}^{-|\phi|^2 + a\phi + b\overline{\phi}}\, \frac{\mathrm{d}\phi \wedge \mathrm{d}\overline{\phi}}{2\pi \mathrm{i}}$$

After integrating out the fermions, we have

$$Z \propto \int \mathrm{d}\Delta_{\mathrm{x}}\, \mathrm{e}^{-\beta V F_{\mathrm{x}}}$$

where

$$F_{\mathrm{FM}} = \frac{1}{M_{1,1}(0)}\Delta_{\mathrm{FM}}^2 - \sum_{\sigma\in\{+,-\}} \int_p \ln\bigl(1+\sigma\Delta_{\mathrm{FM}} T(p)\bigr)$$

$$F_{\mathrm{dSC}} = \frac{1}{D_{2,2}(0)}|\Delta_{\mathrm{dSC}}|^2 - \int_p \ln\bigl(1+|\Delta_{\mathrm{dSC}}|^2 f_2^2(\boldsymbol{p})\, T(p)\, T(-p)\bigr)$$

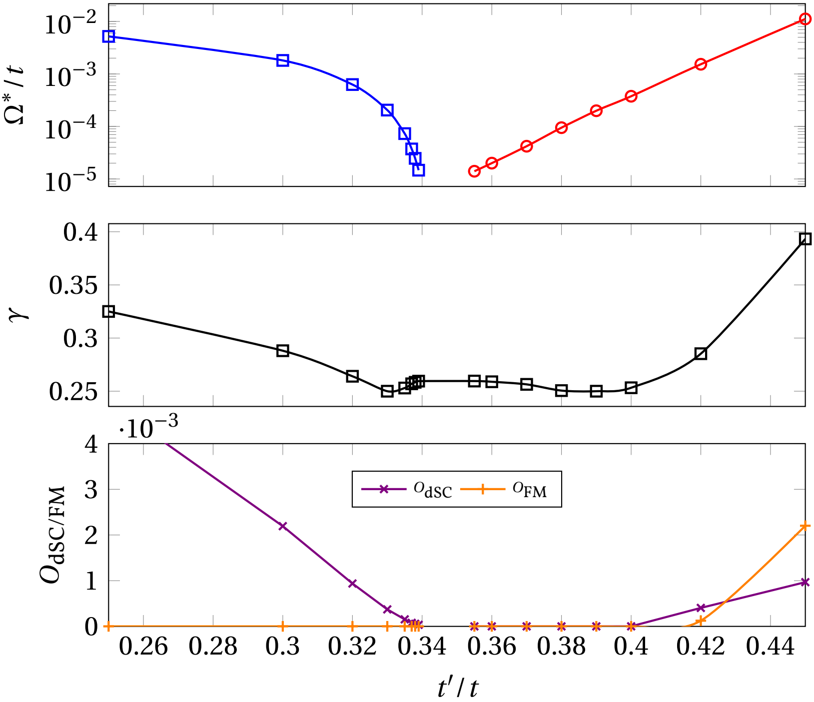
Now we need to minimize the *free energy* as a function of Δ_{x}. At the minimum,

$$O_{\mathrm{dSC}} = 2\Delta_{\mathrm{dSC}}/D_{2,2}(0),\ O_{\mathrm{FM}} = 2\Delta_{\mathrm{FM}}/M_{1,1}(0)$$

where $O_{\mathrm{x}} = \langle \widehat{O}_{\mathrm{x}} \rangle$ with

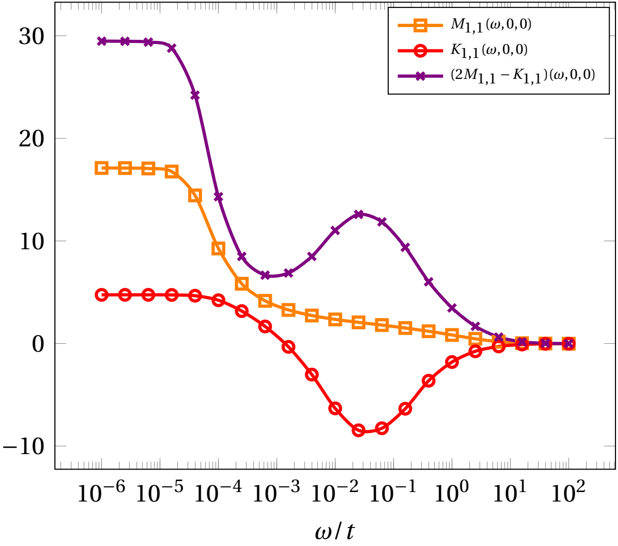
$$\widehat{O}_{\mathrm{FM}} = \int_{k,\sigma} \sigma\, \overline{\Psi}_{k,\sigma} \Psi_{k,\sigma}$$

$$\widehat{O}_{\mathrm{dSC}} = \frac{1}{2}\int_{k,\sigma} \sigma\, f_2(\boldsymbol{k}) \overline{\Psi}_{k,\sigma} \overline{\Psi}_{-k,-\sigma}$$



Ω^* / t
10^{-2}
10^{-3}
10^{-4}
10^{-5}
γ
0.4
0.35
0.3
0.25
$\cdot 10^{-3}$
$O_{\mathrm{dSC/FM}}$
4
3
2
1
0
O_{dSC}
O_{FM}
0.26
0.28
0.3
0.32
0.34
0.36
0.38
0.4
0.42
0.44
t' / t

Density-Density Interaction at the QCP $\left(U + (2M_{1,1} - K_{1,1})(\omega, 0, 0)\right)$
There is a peak at some finite frequency $\tilde{\omega}$



$$F(\lambda) = \int_\gamma f(z)\, \mathrm{e}^{\lambda S(z)}\, \mathrm{d}z \ .$$

If S has a single simple saddle point at an interior point z_0 of the integration contour γ, then the $\lambda \to \infty$ asymptotic of $F(\lambda)$ is given by

$$F(\lambda) = \sqrt{\frac{2\pi}{-S''(z_0)}}\, \lambda^{-1/2}\, \mathrm{e}^{\lambda S(z_0)} \left(f(z_0) + \mathcal{O}\left(\lambda^{-1}\right) \right) .$$

Hence the saddle-point method consists of a *topological* part, which is finding a suitable contour γ which may not exist, and an *analytic* part which involves the evaluation of the asymptotic behavior of the Laplace transform $F(\lambda)$.

Applied to Hubbard-Stratonovich transformation we obtain

$$
\begin{aligned}
\mathrm{e}^{a^2/4} &= \frac{1}{\sqrt{\pi}} \int_{\mathbb{R}} \mathrm{e}^{-(\phi+\mathrm{i}\,c)^2+(\phi+\mathrm{i}\,c)a}\, \mathrm{d}\phi \\
\mathrm{e}^{ab} &= \int_{\mathbb{C}} \mathrm{e}^{-(\phi+\mathrm{i}\psi)(\overline{\phi}+\mathrm{i}\overline{\psi})+a(\phi+\mathrm{i}\psi)+b(\overline{\phi}+\mathrm{i}\overline{\psi})}\, \frac{\mathrm{d}\phi\wedge\mathrm{d}\overline{\phi}}{2\pi\,\mathrm{i}}
\end{aligned}
$$

where $c \in \mathbb{R}$ and $\psi \in \mathbb{C}$ are arbitrary but only for an adequate choice the integrals can be evaluated in saddle-point approximation.

Action with a density-density interaction K:

$$S(\widetilde{\psi},\psi) = -\int_{\omega \boldsymbol{p} s} \overline{\psi}_{\omega \boldsymbol{p} s}(\mathrm{i}\omega - \epsilon_{\boldsymbol{p}} + \mu)\psi_{\omega \boldsymbol{p} s} + \frac{1}{4}\int_p K(p) S^{(0)}(p) S^{(0)}(-p)$$

Integrating out the fermions leads to the free-energy,

$$\begin{aligned}
F = & \frac{\Phi_0^2}{|K(0)|} + 2\sum_{p>0} \frac{\Phi(p)\widetilde{\Phi}(p)}{|K(p)|} \\
& - \frac{2}{\beta V} \ln\det\Big[\big(\mathrm{i}\, p_0 - \epsilon_{\boldsymbol{p}} + \mu + \mathrm{i}\, I_K(0)\Phi_0\big)\delta_{p,p'} \\
& \qquad - \mathrm{i}\big(I_K(p-p')\Phi(p-p')\Theta(p-p'>0) \\
& \qquad + I_K(p'-p)\widetilde{\Phi}(p'-p)\Theta(p'-p>0)\big)\Big]_{p,p'} + C
\end{aligned}$$

$\Phi_0 = \phi_0 + \mathrm{i}\psi_0$ with $\phi_0, \psi_0 \in \mathbb{R}$ and for $p > 0$,
$\Phi(p) = \phi(p) + \mathrm{i}\psi(p), \widetilde{\Phi}(p) = \overline{\phi}(p) + \mathrm{i}\overline{\psi}(p)$ with $\phi(p), \psi(p) \in \mathbb{C}$.
$I_f(x) = 1 \quad \text{if} \quad f(x) \geq 0 \quad \text{else} \quad \mathrm{i} \quad \text{for} \quad f(x) \in \mathbb{R}$.

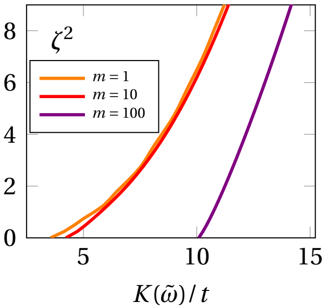
We make the following ansatz for Φ,

$$\Phi(p) = \Phi_{\tilde{\omega}} \delta_{p_0,\tilde{\omega}} \,,$$
$$\widetilde{\Phi}(p) = \widetilde{\Phi}_{\tilde{\omega}} \delta_{p_0,\tilde{\omega}} \,.$$

So in addition to the static field Φ_0 at zero frequency the free-energy depends on $\Phi_{\tilde{\omega}}$ and $\widetilde{\Phi}_{\tilde{\omega}}$, which incorporates a dependence on K at the finite frequency $\tilde{\omega}$.
The free-energy now reads

$$F = \frac{\Phi_0^2}{|K(0)|} + 2\frac{\Phi_{\tilde{\omega}} \widetilde{\Phi}_{\tilde{\omega}}}{|K(\tilde{\omega})|} - \frac{2}{\beta \mathrm{V}} \sum_{\boldsymbol{p}} \ln\det \Big[(\mathrm{i}\, p_0 - \epsilon_{\boldsymbol{p}} + \mu + \mathrm{i}\, I_K(0)\Phi_0)\delta_{p_0,p_0'} - \mathrm{i}\, I_K(\tilde{\omega}) \Big(\Phi_{\tilde{\omega}}\, \delta_{p_0-p_0',\tilde{\omega}} + \widetilde{\Phi}_{\tilde{\omega}}\, \delta_{p_0'-p_0,\tilde{\omega}} \Big) \Big]_{p_0,p_0'} + C \,.$$

Let $\zeta = \left|\Phi_{\tilde{\omega}}\widetilde{\Phi}_{\tilde{\omega}}\right|^{1/2}$ at the saddle point of the free-energy.
$(\tilde{\omega} = \frac{2\pi}{\beta}m)$

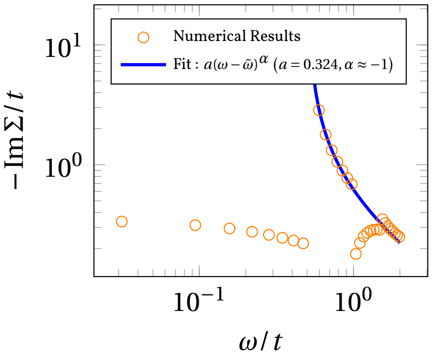


The fermionic propagator is then given by the diagonal of

$$G = \left[(\mathrm{i}\,p_0 - \epsilon_{\boldsymbol{p}})\delta_{p,p'} + \zeta\left(\delta_{p_0-p_0',\tilde{\omega}} + \delta_{p_0'-p_0,\tilde{\omega}}\right)\right]^{-1}_{p,p'} =$$

$$\left[\delta_{p_0,p_0'} + \zeta\frac{\left(\delta_{p_0-p_0',\tilde{\omega}} + \delta_{p_0'-p_0,\tilde{\omega}}\right)}{\sqrt{\mathrm{i}\,p_0 - \epsilon_{\boldsymbol{p}}}\sqrt{\mathrm{i}\,p_0' - \epsilon_{\boldsymbol{p'}}}}\delta_{\boldsymbol{p},\boldsymbol{p'}}\right]^{-1}_{p,p'} \cdot \left[\frac{\delta_{p,p'}}{\sqrt{\mathrm{i}\,p_0 - \epsilon_{\boldsymbol{p}}}\sqrt{\mathrm{i}\,p_0' - \epsilon_{\boldsymbol{p'}}}}\right]_{p,p'}$$

Imaginary part of the Dyson self-energy computed for $\zeta = 0.5$. The plot shows only the low frequency regime when $\epsilon = 0$.

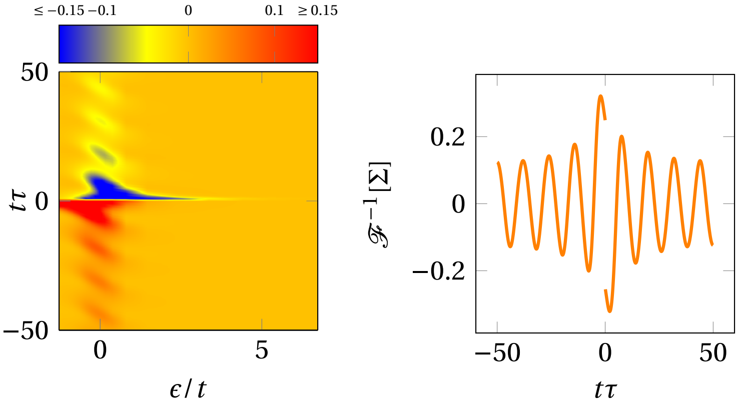


Close to the Fermi surface and for small frequencies the full propagator behaves as

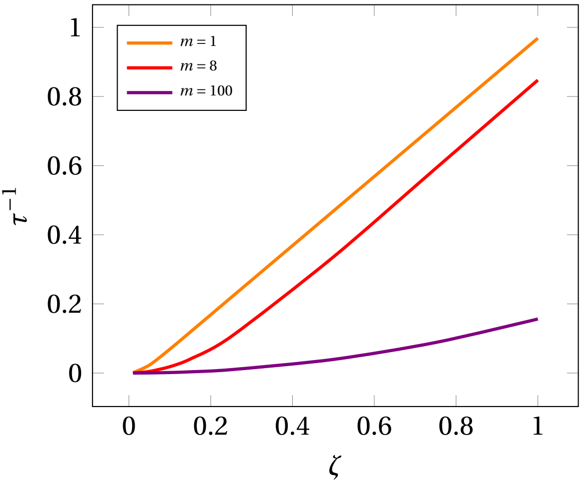
$$g \approx \frac{1}{\mathrm{i}\omega - \epsilon_p + \mathrm{i}\,\mathrm{sgn}(\omega)\tau^{-1}}$$

where τ can be interpreted as the quasiparticle lifetime.

Inverse Fourier transform of the full propagator and the self-energy



Quasiparticle lifetime



Summary

- NFLL self-energy suppresses gap formation
- There is a QCP in the 2D-Hubbard model at $t'/t = 0.341$ at vHF
- Mean-field approximations in the density-density channel require some special considerations.
- The frequency dependence of the density-density interaction leads to short quasiparticle lifetime.