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Timescale of magnetic fluctuations across and above the Mott transition

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FERMI FÉDÉRATION DE RECHERCHE MATIÈRE ET INTERACTIONS

UNIVERSITÉ TOULOUSE III PAUL SABATIER

Laboratoire de Chimie et Physique Quantiques

Erasmus+

Outline

Outline

Introduction

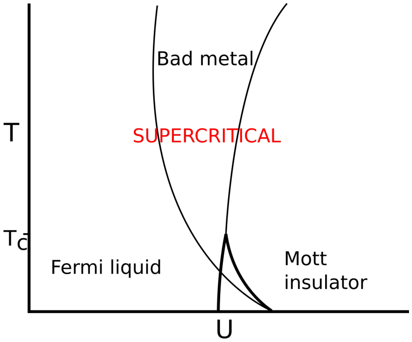

Figure 1 – Cartoon picture of the DMFT phase diagram of the half-filled Hubbard model

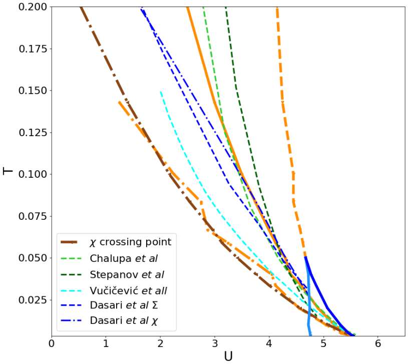

Figure 2 – DMFT phase diagram of the half-filled Hubbard model using previously defined crossover lines [1-5]

Introduction

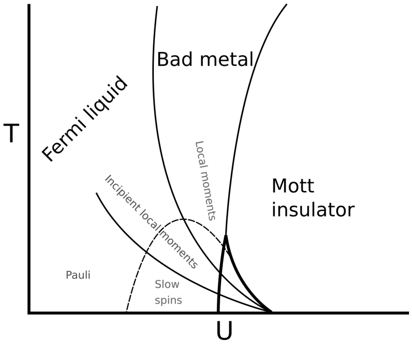

Figure 3 – Cartoon picture of the DMFT phase diagram of the half-filled Hubbard model

We propose a **new characterization** of the phase diagram using only **timescales of magnetic fluctuations** and **valence fluctuations** that brings :

- Physical insight to the crossover lines in the supercritical region
- New "slow spin" dome in the Fermi liquid regime.

Gaspard, L. ; Tomczak, J. M. Timescale of local moment screening across and above the Mott transition, 2021 https ://arxiv.org/abs/2112.02881v1

Outline

The Hubbard model on the Bethe lattice ($Z = \infty$)

- One orbital per site (i)
- Half-filling (one electron per site i)
- t : nearest neighbor hopping
- U : Coulomb repulsion between electrons on the same site
- $Z = \infty$ Bethe lattice with the density of states : $D(\varepsilon) = \frac{\sqrt{4t^2-\varepsilon^2}}{2\pi t^2}$

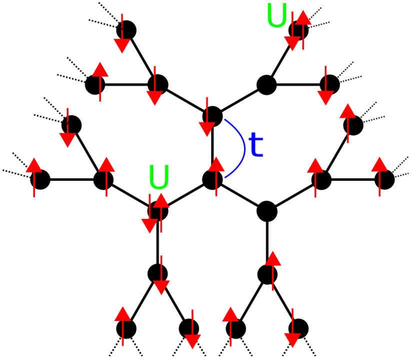

Figure 4 – Schematic picture of the Hubbard model on a Z=3 Bethe lattice

$$\hat{H} = -t \sum_{\langle i,j \rangle,\sigma} \hat{c}^{\dagger}_{i,\sigma} \hat{c}_{j,\sigma} + U \sum_{i} \hat{n}_{i,\uparrow} \hat{n}_{i,\downarrow} \quad (1)$$

DMFT on the Bethe lattice ($Z = \infty$)

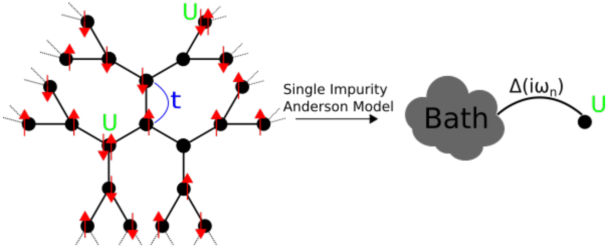

Figure 5 – Schematic picture of the Single Impurity Anderson Model (SIAM)

We replace the Bethe lattice by the SIAM :

$$\hat{H} = \hat{H}_{\text{atom}} + \hat{H}_{\text{bath}} + \hat{H}_{\text{hybridization}}$$

$$\hat{H} = U\hat{n}_\uparrow\hat{n}_\downarrow + (\varepsilon_0 - \mu)(\hat{n}_\uparrow + \hat{n}_\downarrow) + \sum_{l,\sigma} \varepsilon_l \hat{a}^\dagger_{l,\sigma}\hat{a}_{l,\sigma} + \sum_{l,\sigma} V_l(\hat{a}^\dagger_{l,\sigma}\hat{c}_\sigma + \hat{c}^\dagger_\sigma \hat{a}_{l,\sigma})$$

DMFT on the Bethe lattice (Z=∞) is **exact** :

$$\Sigma_{\text{imp}}(\omega)$$

CT-HYB: $\Delta(\omega) = t^2 G_{\text{imp}}(\omega) \rightarrow \Sigma_{\text{imp}}(\omega)$

$\Sigma_{\text{imp}}(\omega) \rightarrow G_{\text{loc}}(\omega)$

$$G_{\text{loc}}(\omega) = \int \mathrm{d}\varepsilon \frac{1}{\omega-\varepsilon-\Sigma_{\text{imp}}(\omega)} D(\varepsilon)$$

$G_{\text{imp}}=G_{\text{loc}}$: $G_{\text{loc}}(\omega) \rightarrow \Delta(\omega) = t^2 G_{\text{imp}}(\omega)$

CT-HYB : Expansion of the partition function in the interaction representation and Monte-Carlo integration

$$Z = \text{Tr}\left[\mathcal{T}_\tau \exp\left(-\beta(\hat{H}_{\text{atom}} + \hat{H}_{\text{bath}})\right) \exp\left(-\int_0^\beta \mathrm{d}\tau \hat{H}_{\text{hybridization}}(\tau)\right)\right]$$

Magnetic susceptibility

We are interested in the **local magnetic susceptibility** computed in imaginary time τ :

$$\chi_m(\tau) = g^2 \left\langle \mathcal{T}_\tau \hat{S}_z(\tau)\hat{S}_z(0) \right\rangle \quad (2)$$

From this we can get the **static local magnetic susceptibility** :

$$\chi_m(i\omega = 0) = \int_0^\beta \chi_m(\tau)\mathrm{d}\tau \quad (3)$$

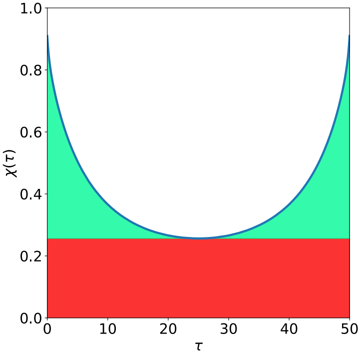

Figure 6 – Local magnetic susceptibility in imaginary time for U=4.9 and $\beta = 50$

$$\chi_m(i\omega = 0) = \beta\chi_m\left(\tau = \frac{\beta}{2}\right) + \int_0^\beta \chi_m(\tau) - \chi_m\left(\tau = \frac{\beta}{2}\right)\mathrm{d}\tau \quad (4)$$

Magnetic susceptibility

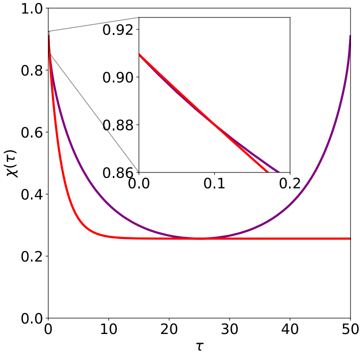

Figure 7 – Local magnetic susceptibility for U=4.9 and $\beta = 50$

Fit of $\chi(\tau)$ for τ close to 0 :

$$\chi_m\left(\tau \ll \frac{\beta}{2}\right) = \chi_m\left(\tau = \frac{\beta}{2}\right) + \left[\chi_m(\tau = 0) - \chi_m\left(\tau = \frac{\beta}{2}\right)\right] e^{-\frac{\tau}{t_m}} \quad (5)$$

t_m is the **timescale of the magnetic fluctuations**

Outline

Evolution of t_m through the phase diagram

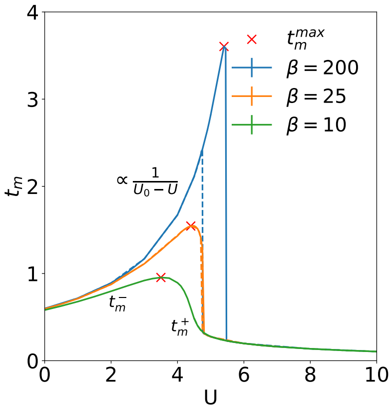

Figure 8 – t_m as a function of the interaction U for three values of β

- At low temperature (**high** β) : discontinuity in t_m at the phase transition.
- At high temperature (**low** β) : continuous evolution of t_m
- In all cases : t_m reaches a maximum for a value of U

Evolution of t_m through the phase diagram

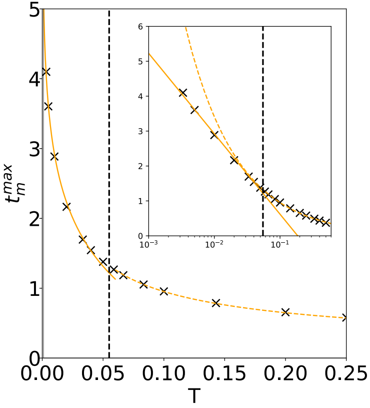

Figure 9 – Value of the maximum of t_m at constant U as a function of the temperature

$t_m^{max}(T)$ changes behavior for a given temperature $T_c \approx 0.055$

- **Below** T_c :
  t_m^{max} exhibits a logarithmic behavior : $t_m^{max} \approx -\log\left(\frac{T}{\gamma}\right)$, $\gamma \approx 0.19$
- **Above** T_c :
  t_m^{max} behaves as a power : $t_m^{max} \propto T^{-\alpha}$, $\alpha \approx 0.27$

Phase diagram using the timescales

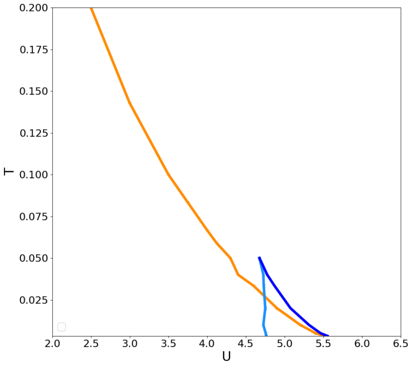

Figure 10 – Phase diagram of the Hubbard model using previously defined quantities

- The coexistence region is reproduced using the **discontinuity in t_m**
- The orange line is the coordinate of the **maximum** of t_m (t_m^{max}). It separates the Fermi liquid (where the magnetic fluctuations timescale increases with the effective mass of the quasiparticle) and the Bad metal (where the magnetic fluctuations become slower).

Phase diagram using the timescales

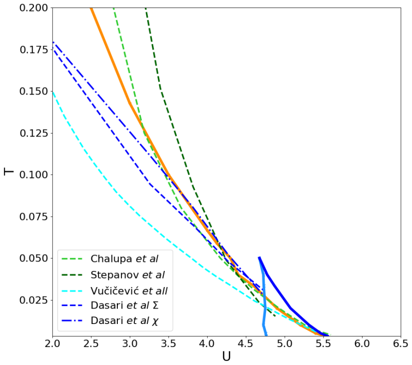

Figure 11 – Comparison the t_m^{max} line from our work with previous works

- The coexistence region is reproduced using the **discontinuity in t_m**
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Evolution of t_m through the phase diagram

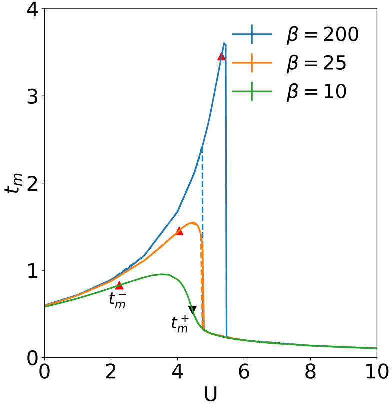


Figure 12 – t_m as a function of the interaction U for three values of β

- First inflection point of t_m (▲), exists in all the cases : formation of a local moment.
- Second inflection point of t_m (▼), exists only when t_m is continuous : reaching the atomic limit.

Phase diagram using the timescales

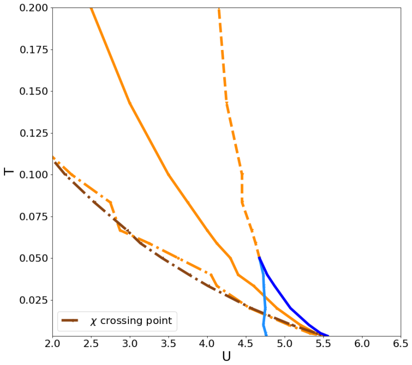


Figure 13 – Comparison the t_m^{max} line from our work with previous works

- The t_m^- line is consistent with the crossover line between $\chi^{\text{local-moment}}$ and χ^{dynamic} indicating the predominance of the local moment.
- The t_m^+ line indicates the end of the crossover between the bad insulator and the Mott phase as the growing interaction has less and less effect on the magnetic fluctuations period (reaching the atomic limit).

Phase diagram using the timescales

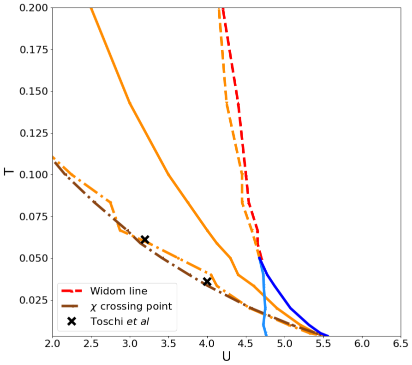


Figure 14 – Comparison the t_m^{max} line from our work with previous works

- The t_m^- line is consistent with the crossover line between $\chi^{\text{local-moment}}$ and χ^{dynamic} indicating the predominance of the local moment.
- The t_m^+ line indicates the end of the crossover between the bad insulator and the Mott phase as the growing interaction has less and less effect on the magnetic fluctuations period (reaching the atomic limit).

Valence fluctuations

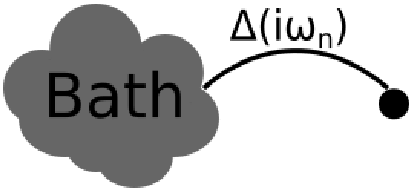


Figure 15 – Schematic representation of a site coupled to a bath

One can define the **timescale associated with the valence history** using the DMFT hybridization function $\Delta(i\omega_n)$

$$t_{hyb} = -\frac{1}{\lim\limits_{i\omega_n \to 0} \Im\Delta(i\omega_n)} \tag{6}$$

How do the two different timescales compare ?

Magnetic screening vs valence fluctuations

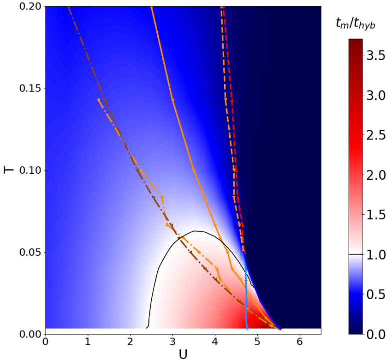


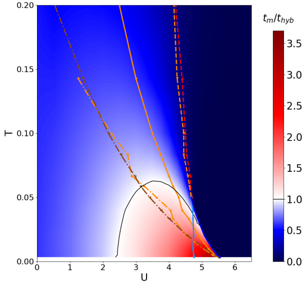
Figure 16 – Heatmap of the ratio between t_m and t_{hyb} in the DMFT phase diagram of the Hubbard model

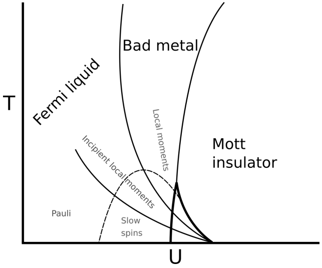
- $t_m/t_{hyb} < 1$: Magnetic fluctuations **faster** than valence fluctuations.
- $t_m/t_{hyb} > 1$: Magnetic fluctuations **slower** than valence fluctuations.
- **Mott phase** : No valence fluctuations, $t_m \ll t_{hyb}$
- **Low interaction** and/or **high temperature** : $t_m < t_{hyb}$
- Appearance of a **dome** where $t_{hyb} > t_m$: valence fluctuations faster than magnetic fluctuations (adiabatic spin response).

Outline

Conclusion

- We provided a **new insight into the phase diagram of the Hubbard model** through the lens of **spin dynamics**.
- We identified a **new crossover line** within the Fermi liquid phase with a region with preponderant local moment
- We identified a regime in which the **spin dynamics is adiabatic**





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