Application of the Finite-Momentum Pairing Method

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?? introduced the method of enforcing a finite momentum on the order parameter to gain access to the coherence length ξ_0 and the London penetration depth $\lambda_{L,0}$. In this chapter, it will be applied in two ways: in section 1.1 on the mean-field level as introduced in **??** on the decorated graphene model, see **??**. Here, the influence of the quantum geometry on superconductivity as explained in **??** will be explored.

In section 1.2, is is applied to the one-band Hubbard model on a square lattice, both on the mean-field level and using Dynamical Mean Field Theory (DMFT) as introduced in **??**. DMFT gives the opportunity to explore the BCS-BEC crossover phenomenon and the simpler model is an opportunity to compare the results from DMFT and Bardeen-Cooper-Schrieffer (BCS) theory.

1.1 BCS: Decorated graphene Model

In BCS theory, the method involves self-consistently solving the gap equation for a set of external parameters, which in the case of the decorated graphene model are the Hubbard interaction U, the hybridization V as well as temperature T and Cooper pair momentum $\mathbf{q}$. This gives gap values Δ_α for the three orbitals $\alpha \in \{\mathrm{Gr_A}, \mathrm{Gr_B}, \mathrm{X}\}$.

Critical Temperatures

The zero-temperature lengths $\xi_0, \lambda_{L,0}$ are extracted from the temperature dependence $\xi(T), \lambda_L(T)$, for example

$$\xi(T) = \xi_0 \left(1 - \frac{T}{T_\mathrm{C}}\right)^{-\frac{1}{2}} \, . \tag{1.1}$$

This means the first step in the analysis is to find the critical temperature T_C. Finding T_C directly by

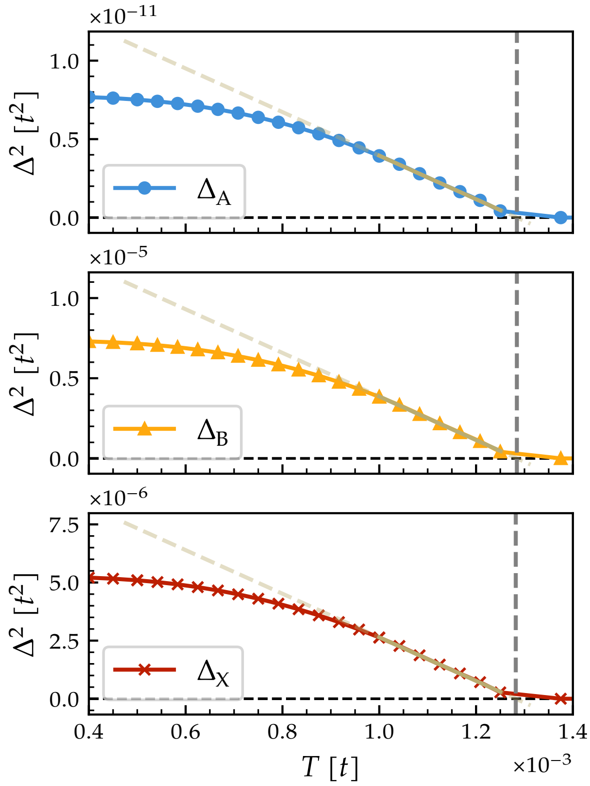

Figure 1.1 – Extraction of T_C from the linear behavior of the order parameter. Shown is the square of the gap Δ_α near T_C for $U = 0.01t$ and $V = 1.6t$. The linear fit for extracting T_C is shown in tan, the corresponding T_C is marked by the dashed gray line.

Instead, it can be extracted from the linear behavior of the order parameter near T_C, see **??**:

$$|\Delta_\alpha|^2 \propto T_C - T \,. \tag{1.2}$$

For a specific U and V, this is shown in fig. 1.1. Notable here is that even though Δ_A is order of magnitude smaller than Δ_B and Δ_X, T_C is the same for every orbital.

Figure 1.2 shows the extracted T_C and gaps against the hybridization V. T_C follows the maximal value of the Δ_α, switching over from X to $\mathrm{Gr_B}$ at $V = 1.44t$. The value of Δ_α exactly follows the orbital weight w_α of the flat band, for the orbitals $\alpha \in \{\mathrm{Gr_A}, \mathrm{Gr_B}, \mathrm{X}\}$. In contrast to a repulsive Hubbard interaction [1] there is no gap closure for a medium V, instead there is just a minimum of the maximal gap value.

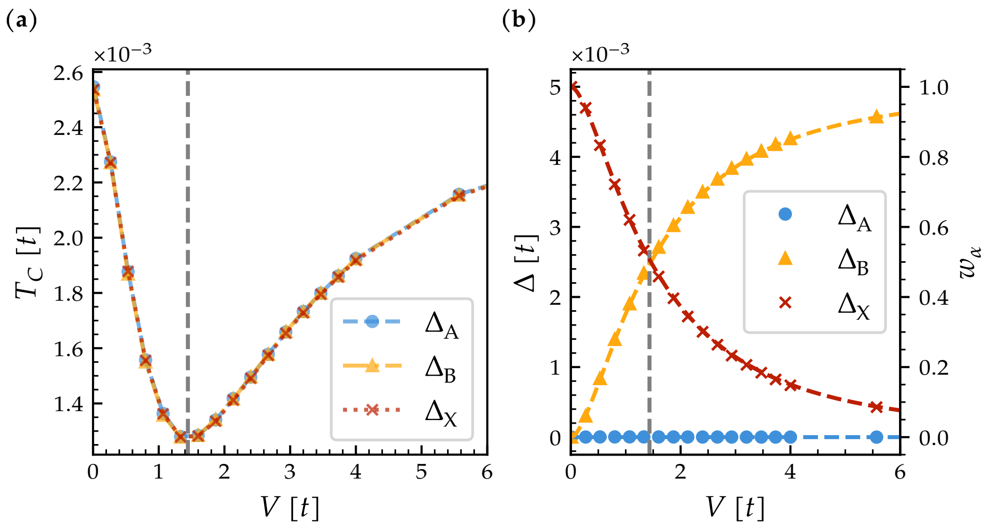

Figure 1.2 – Critical temperatures and gaps against V. (**a**) T_C against hybridization V, the same for all three orbitals. (**b**) Gaps Δ_α for the same values of V. The dashed lines are the orbital weight of the flat band as defined in **??**. The dashed value $V = 1.44t$ is taken from the minimum of $T_C(V)$, coinciding with the switchover of the orbital character. Both plots are for the same $U = 0.01t$.

Extracting the Superconducting Length Scales

The correlation length $\xi(T)$ is associated with the breakdown of the order parameter:

$$|\Psi_{\mathbf{q}}|^2 = |\Psi_0|^2 \left(1 - \xi(T)^2 q^2\right) , \tag{1.3}$$

which means that the q_C where the order parameter breaks down is related to the correlation length via

$$\xi = \frac{1}{q_C} . \tag{1.4}$$

The momentum $\mathbf{q}$ is chosen as $\mathbf{q} = x \cdot \mathbf{b}_1$ with the reciprocal vector $\mathbf{b}_1$ and $x \in [0, 0.5]$. For $x > 0.5$, the Similar to finding T_C, numerical calculations near the point where the gap goes to zero are hard to converge, so instead the

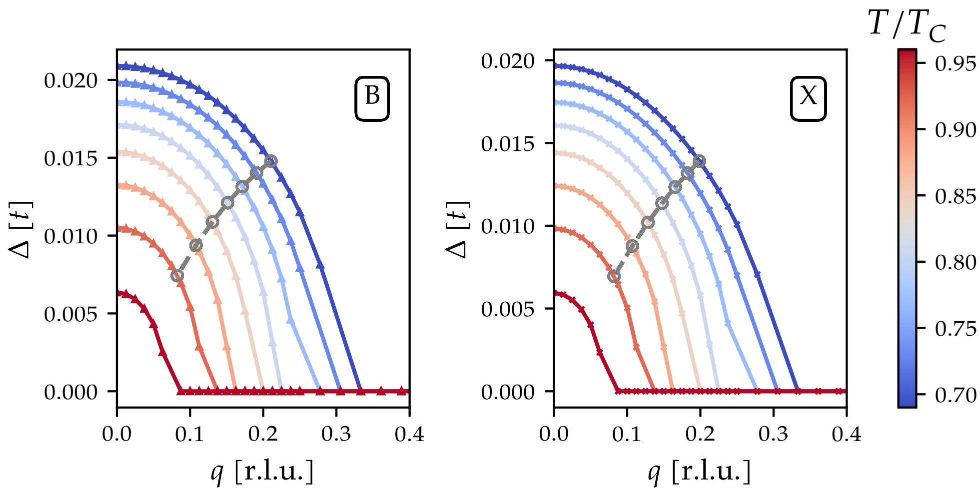

Figure 1.3 – Suppression of the order parameter with q for $V = 1.5t$ **and** $U = 0.1t$**.** The x-axis is marked in relative lattice units, i.e. $\mathbf{q} = q \cdot \mathbf{b}_1$ for the reciprocal unit vector $\mathbf{b}_1$. Marked in gray are the points at which the gaps have fallen off to $1/\sqrt{2}$ of their value at $\mathbf{q} = 0$.

criterion employed here is to choose $\mathbf{Q}$ such that

$$\left|\frac{\psi_{\mathbf{Q}}(T)}{\psi_0(T)}\right| = \frac{1}{\sqrt{2}}\,, \tag{1.5}$$

and then take

$$\xi = \frac{1}{\sqrt{2}\mathbf{Q}}\,, \tag{1.6}$$

compare ref. [2] for discussion about this method and comparison to other ways to extract the superconducting length scales from the $\mathbf{q}$-dependence of the order parameter.

As shown in fig. 1.2b, only Δ_{B} and Δ_{X} have a significant contribution in the parameter range of U here, so for these the $\mathbf{q}$-dependence is shown in fig. 1.3 for $V = 1.5$, so in a parameter regime switching over between dominating X and B contribution. For higher temperatures $q_C \to 0$, showing how the correlation length diverges for $T \to T_{\mathrm{C}}$.

In the case of high and low V where the superconducting order is dominated by one of $\Delta_{\mathrm{A}}, \Delta_{\mathrm{X}}$, fig. 1.4 shows that the gap does not fully go down to 0 for

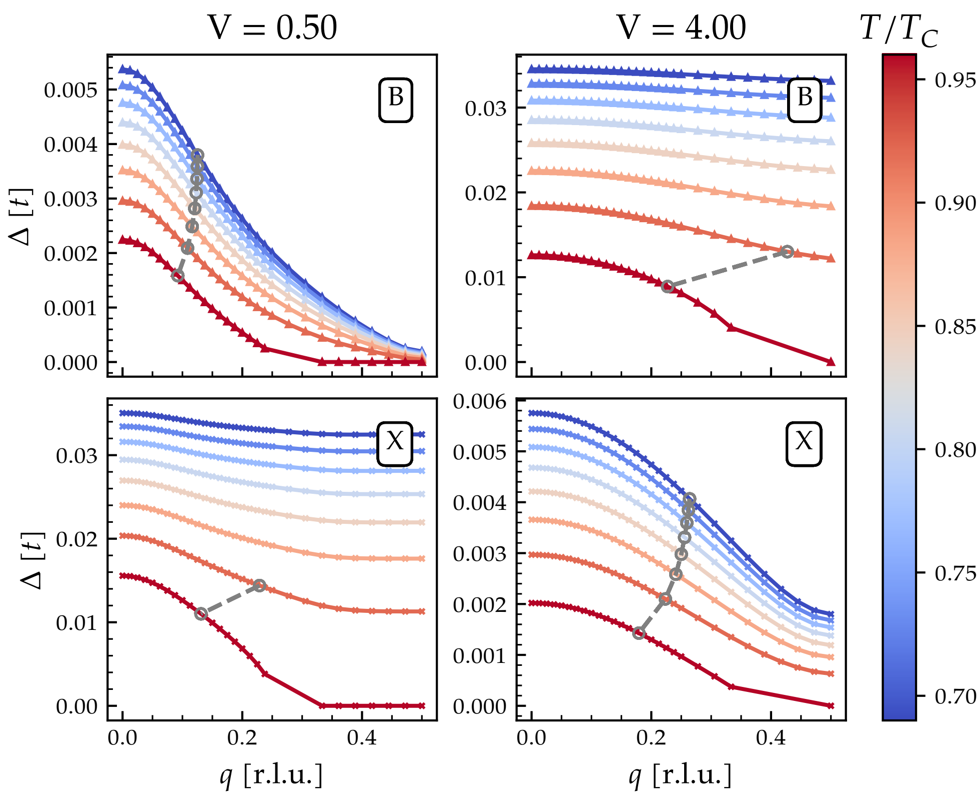

Figure 1.4 – Suppression of the order parameter with q for $V = 0.5t$ **and** $V = 4t$ **(both for** $U = 0.1t$**).** In contrast to fig. 1.3, in this parameter regime the order parameter does not get fully suppressed for the maximal $q = 0.5$.

$\mathbf{q} = {}^1\!/_2 \cdot \mathbf{b}_1$, meaning that the correlation length is smaller than

$$\xi = \frac{1}{0.5 \cdot |\mathbf{b}_1|} = \frac{\sqrt{3}a}{2\pi} = \frac{a_0}{2\pi} \,. \tag{1.7}$$

Besides the correlation lengths extracted from the behavior of the order parameter against $\mathbf{q}$, also the behavior of the superconducting current $j(\mathbf{q})$ is

Talk about limitation of GL: does not apply for high q

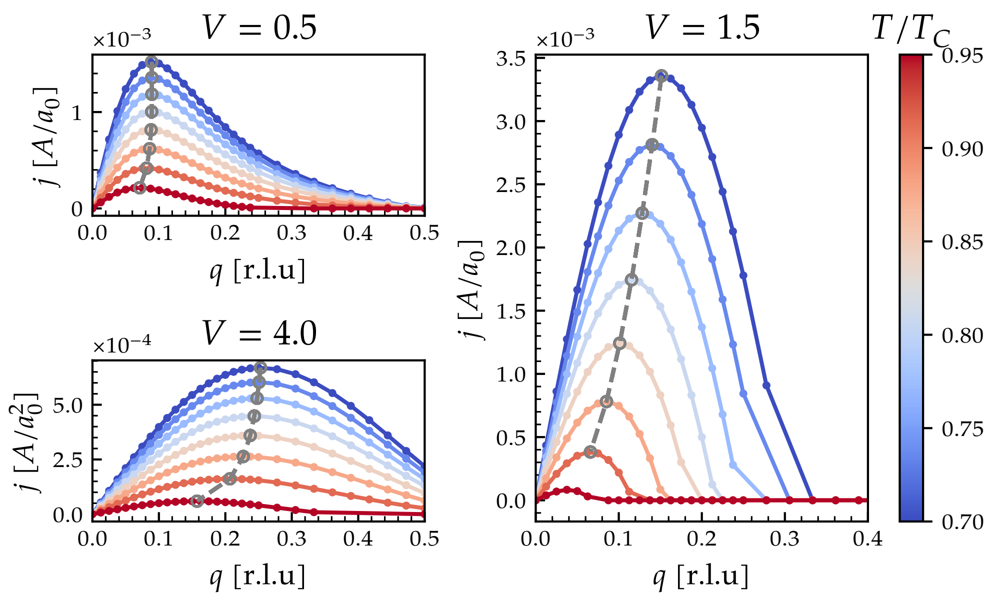

Figure 1.5 – Superconducting current from a finite q. For calculation of the London penetration depth λ_{L}, the maximum j_{dp} of the current is needed, marked here in gray.

needed to calculate the London penetration depth λ_{L} via

$$\lambda_{\mathrm{L}}(T) = \sqrt{\frac{\Phi_0}{3\sqrt{3}\pi\mu_0\xi(T)j_{dp}(T)}}\,. \tag{1.8}$$

In particular, the maximum j_{dp} (the depairing current) is used. Figure 1.5 shows the current $\mathbf{j}(\mathbf{q})$ with the maximum calculated from an interpolation marked for every temperature. As in the $\mathbf{q}$-dependence of the gaps, for the low and high V-values, the current is not fully suppressed for the lower temperatures and $q = 0.5$. In contrast to the analysis of the gaps, it is still possible to find a maximum of the current in theses cases, but because the validity of Ginzburg-Landau theory is not given for high $\mathbf{q}$, it is unclear whether the connection to the superconducting length scales as derived in Ginzburg-Landau theory is given.

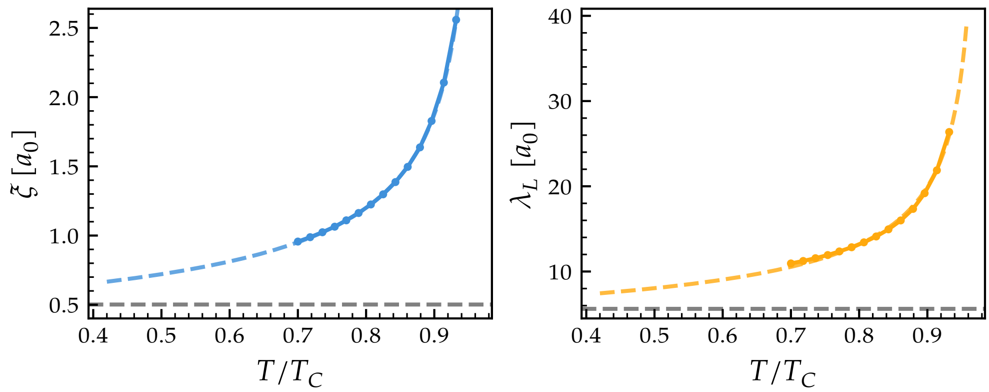

Figure 1.6 – Temperature dependence of the correlation length ξ and London penetration depth λ_L for $V = 1.50t$ and $U = 0.1t$. The fits for extracting the zero-temperature values ξ_0, $\lambda_{\mathrm{L},0}$ are marked as dash lines.

Figure 1.6 shows the temperature dependence for $\xi(T)$ and λ_L. These can be fit to

$$\xi(T) = \xi_0 \left(1 - \frac{T}{T_\mathrm{C}}\right)^{-\frac{1}{2}} \tag{1.9}$$

and

$$\lambda_\mathrm{L}(T) = \xi_0 \left(1 - \frac{T}{T_\mathrm{C}}\right)^{-\frac{1}{2}} \tag{1.10}$$

to obtain the zero-temperature values ξ_0 and $\lambda_{\mathrm{L},0}$. For the low and and high V (fig. 1.4): extraction of $xi(T)$ is not properly possible due to the behaviour of the gaps against q. One can try to extract information from the criterium, but the temperature dependence does not follow the fit.

Make that properly

Length Scales

Figure 1.7 shows the extracted length scales for two different values of the attractive interaction U. In the coherence length, the behavior is similar for between these two values: the orbital with the largest gap value has the shortest coherence length, with a switchover between the small and large V-values. In

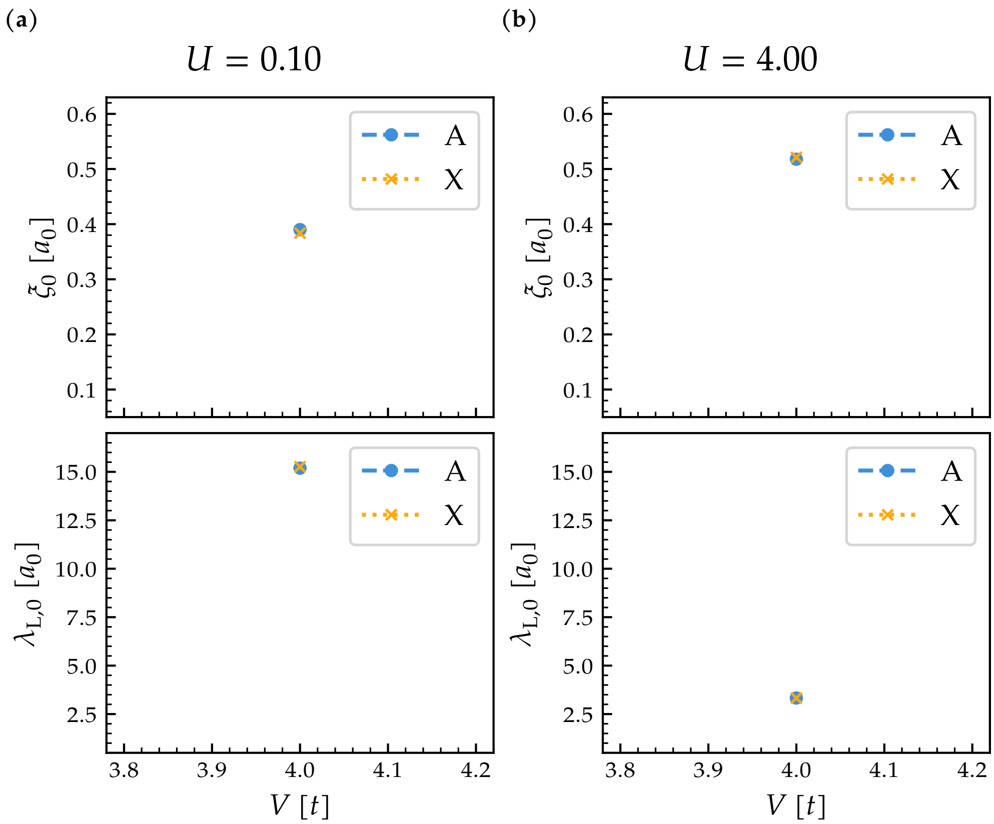

Figure 1.7 – Superconducting length scales for $U = 0.1t$**.** The coherence length ξ_0 is related to the size of electron pairs, the London penetration depth $\lambda_{L,0}$ is the distance magnetic fields penetrate into the material.

general, a higher attractive interaction is associated with smaller Cooper pairs. Interestingly, the orbital with vanishing gaps in the large V-limit go to the same value of ξ_0, independent of U. It should be noted however that for the B-orbital, the coherence length becomes smaller than $\frac{a_0}{2\pi} \approx 1.6$, the minimum value that can be extracted for $V \approx 3$, so no statement about the dominating gap can be made in the large V-limit.

Talk about the exact moment of the switchover

Talk about London penetration depth

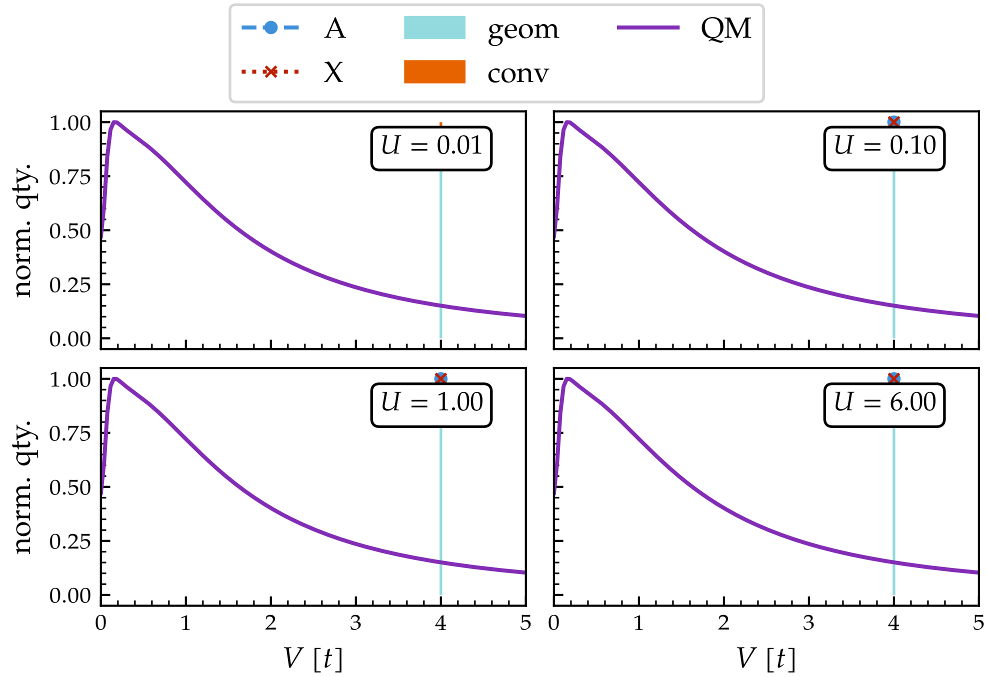

Figure 1.8 – Comparison of the superfluid weight calculated by different methods. All quantities are normalized to analyze the general trend in comparison to the quantum metric. For the calculation coming from linear response theory (see **??**), the geometric and conventional contributions are marked separately.

From the London penetration depth $\lambda_{\mathrm{L},0}$, the superfluid weight can be calculated via

$$D_S \propto \lambda_{\mathrm{L},0}^{-} \tag{1.11}$$

Another way to calculate the superfluid weight from linear response theory was shown in **??**. Figure 1.8 shows the superfluid weight from the **q**-dependence and the linear response formula, split up between the geometric and the conventional contribution as well as the quantum metric. The calculation from the linear response formula shows that the isolated flat band limit, where the geometric contribution dominates the superfluid weight is only given for low U, when it is on the order of the gap between the flat and dispersive bands. For

$U = 1.00t$, the conventional contribution becomes bigger, while for $U = 6.00t$ it dominates up until the gap (which is given by V) is comparable to U.

Where is the maximum of qm, compared with maximum of Aalto DS

The results from the Finite Momentum Pairing (FMP) method agree with the linear response insofar that they show a peak in the intermediate V-regime and go to zero for $V \to 0$ and $V \to \infty$, but the location of this peak is not the same between the two method. Especially in the low V-limit, the FMP method (at least for this model) is at the boundary of applicability, so this is possibly a limitation of the method.

The critical temperatures in BCS theory as seen in fig. 1.2a shows a minimum in the intermediate V region. The effect of D_S that cannot be seen in the critical temperatures from BCS theory, so the expectation would that the critical temperature actually falls off in the low and high V limit and the intermediate region is actually better for superconductivity .

Is that correct?

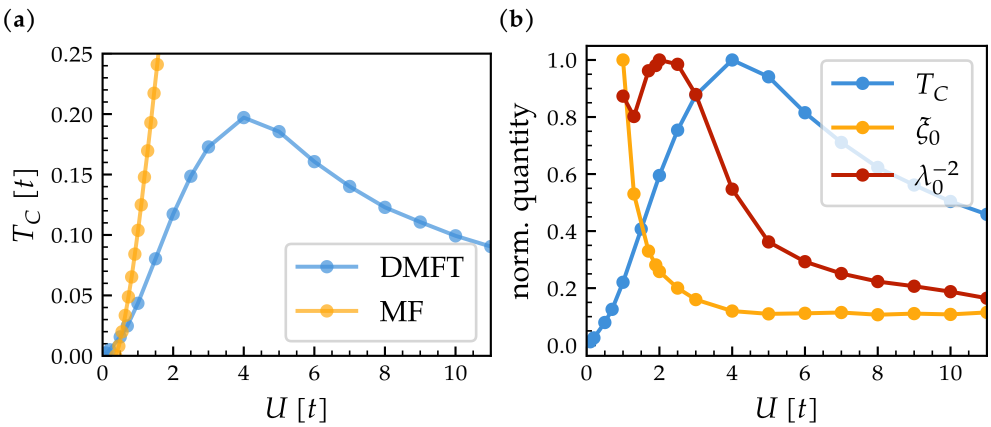

Figure 1.9 – T_C and superconducting length scales for the one-band Hubbard model. (**a**) T_C calculated from mean-field theory and DMFT respectively. It shows the characteristic dome of the BCS-BEC crossover that is not captured in mean-field theory. (**b**)

1.2 BCS and DMFT: One-Band Hubbard Model on the Square Lattice

BCS-BEC Crossover

DMFT gives insight into the phenomenon of the BCS-BEC crossover. Can extract T_C same way as above. Figure 1.9a shows T_C against U. The DMFT curve shows the typical dome-shape of the BCS-BEC crossover and the fact that the MF T_C marks the pairing temperature, which is different to the superconducting T_C.

The extraction of the superconducting length scales works the same as in section 1.1. Figure 1.9b shows how these length scales characterize the BCS-BEC crossover phenomenon: the coherence length goes to zero when going into the BEC regime, marking how the Cooper pairs become strongly localized. The superfluid weight has its maximal value for low U and also goes to zero for stronger attractive interaction,

Talk about the fact that the method works for all U values

Minimal value of coherence length?

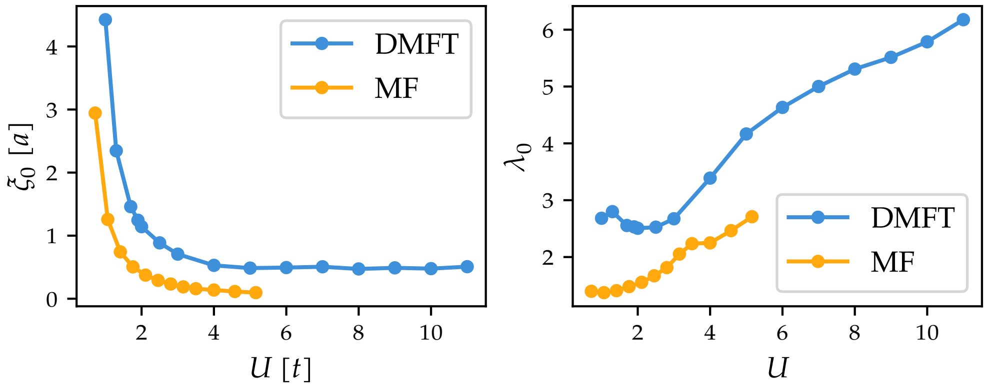

Figure 1.10 – Comparison of superconducting length scales between mean-field and DMFT.

Comparison of MF and DMFT

Figure 1.10 shows that in mean-field theory, the FMP method in BCS theory underestimates the length scales in comparison to the DMFT method.

Write what goes on in the high U limit between MF and DMFT

Why? What is captured in DMFT?