Mott-Hubbard transition in the mass-imbalanced Hubbard model

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Abstract. The mass-imbalanced Hubbard model represents a continuous evolution from the Hubbard to the Falicov-Kimball model. We employ dynamical mean field theory and study the paramagnetic metal-insulator transition, which has a very different nature for the two limiting models. Our results indicate that the metal-insulator transition rather resembles that of the Hubbard model as soon as a tiny hopping between the more localized fermions is switched on. At low temperatures we observe a first-order metal-insulator transition and a three peak structure. The width of the central peak is the same for the more and less mobile fermions when approaching the phase transition, which agrees with our expectation of a common Kondo temperature and phase transition for the two species.

1 Introduction

Strongly correlated electron systems give raise to a plethora of fascinating physics, and the Mott-Hubbard metal-insulator transition [1,2] is one of the prime examples. Here, electronic correlations split the non-interacting band so that an insulating state develops, even for an odd number of electrons per site and even without symmetry breaking in the paramagnetic phase. The arguably first satisfactory modeling of this transition was given by Hubbard in the so-called Hubbard-III approximation [3]. This is a decoupling of the equation of motion for the Green function based on an alloy analogy, which assumes mobile electrons moving in a lattice of immobile electrons. Physically this solution yields separated Hubbard bands at $\pm U/2$ for large interactions $U$, and a continuous metal-insulator transition at a critical interaction strength $U_c$, where both Hubbard bands touch each other, see Figure 1 (left). Upon further reducing $U$, the pseudogap gets filled and eventually the non-interacting density of states (DOS) is recovered [4]. While the Hubbard-III approximation was designed as an approximation for solving the Hubbard model (HM), it already bares the main ingredients of the Falicov-Kimball model (FKM) [5]: mobile and immobile electrons that are coupled through an interaction $U$. Because of this resemblance, Hubbard [3] is sometimes given credit for inventing the FKM.

In particular thanks to insights from dynamical mean field theory (DMFT) [6,7], we nowadays know that the Mott-Hubbard transition in the Hubbard model is more intricate. First of all, it is first order for temperatures below a critical point, as in the van der Waals liquid-vapor transition. Second, when turning metallic, a quasiparticle resonance develops within the, still pronounced, gap. Consequently a three-peak structure emerges, which only dissolves into a single peak at much smaller interaction strength, see Figure 1 (right). In contrast, the FKM shows the Hubbard-III type of metal-insulator transition in DMFT [4,8] as in Figure 1 (left).

1 DMFT spectra for the Falicov-Kimball model have been calculated analytically at $U = 0, 1.5, 2.0, 5.2, D = 2$; those of the Hubbard model have been calculated at $U = 0, 4.0, 5.2, 5.5, D = 2$ using CT-QMC simulations as a DMFT impurity solver and the maximum entropy method.
Since these two metal-insulator transitions are genuinely different, we ask in this paper: what is the nature and the order of the metal-insulator transition when continuously tuning our model from the FKM to the HM at finite temperature?

We address this question by increasing the hopping amplitude of the less mobile fermions from zero (FKM) to the same amplitude as the mobile fermions (HM). As one may construe the different hopping amplitude as a mass difference, one can also perceive this intermediate one may construe the different hopping amplitude as the mobile fermions (HM). As and the order of the metal-insulator transition when continuously different, we ask in this paper: what is the nature and the order of the metal-insulator transition when continuously tuning the model from the FKM to the HM.

The Hamiltonian of the mass-imbalanced Hubbard model for one orbital can be written as:

\[ H = -t_c \sum_{\langle ij \rangle} (\hat{c}_i^\dagger \hat{c}_j + \hat{c}_j^\dagger \hat{c}_i) - t_f \sum_{\langle ij \rangle} (\hat{f}_i^\dagger \hat{f}_j + \hat{f}_j^\dagger \hat{f}_i) + U \sum_i \hat{n}_{c,i} \hat{n}_{f,i}, \]  

(1)

where \( \hat{c}_i^\dagger \) and \( \hat{c}_i \) create and annihilate, respectively, one of the fermion species, while \( \hat{n}_{c,i} = \hat{c}_i^\dagger \hat{c}_i \) and \( \hat{n}_{f,i} = \hat{f}_i^\dagger \hat{f}_i \) are the corresponding occupancy operators at site \( i \). The hopping between next neighbors, \( \langle ij \rangle \), is mediated by the corresponding hopping amplitudes, \( t_c \) and \( t_f \); and it costs the Hubbard interaction \( U \) if there is a \( c \) and \( f \) fermion on the same site.

In the following, we consider a Bethe lattice, i.e., semi-elliptic densities of states \( D_x(\omega) = \frac{2}{\pi D} \sqrt{1 - (\omega/D_x)^2} \) with half bandwidth \( D_x \sim t_f \) for the two fermionic species \( x = c, f \). In the following, we set \( D_c \equiv 2 \) as our unit of energy and vary the mass balance \( D_f/D_c = t_f/t_c \) between 0 and 1.

The two limits of mass imbalance are evident from equation (1): in the case \( D_f/D_c = 0 \), the \( f \) fermions are truly frozen and we arrive at the FKM. On the other hand, if \( D_f/D_c = 1 \), we can identify \( c \) and \( f \) with spin-up and spin-down, respectively, and obtain the mass-balanced HM.

The mass-imbalanced HM (1) can be solved exactly using DMFT, which maps the lattice model self-consistently on a single impurity Anderson model (SIAM) [7]. We use the w2dynamics package [21, 22], which employs CT-QMC in the hybridization expansion [23, 24] to solve the auxiliary SIAM. In order to obtain spectral functions \( A(\omega) \) in real frequency from the imaginary frequency DMFT Green’s function \( G(\omega_n) \), the maximum entropy method (MAXENT) is used [25].

Both in the FKM and HM, the metal-insulator transition is shadowed by an anti-ferromagnetic dome for dimension \( d \geq 3 \). In order to be able to study the Mott transition, we hence enforce the paramagnetic solution and half-filling of both, \( c \) and \( f \) fermions. In the HM, these constraints can be enforced by explicitly symmetrizing over spins and setting the chemical potential to \( \mu = U/2 \), respectively. Away from this HM limit, we again enforce half-filling by fixing \( \mu = U/2 \) such that the total number

\[ \zeta = \frac{(t_c - t_f)}{t_c + t_f} \]  

is used instead of our \( t_f/t_c \).
of fermions per site is $n = 1$. However to ensure the paramagnetic solution at half-filling for both, $c$ and $f$, fermions individually, we symmetrize the hybridization functions in imaginary time: $\Delta(\tau) = \Delta(\beta - \tau)$.

### 3 Results

As mentioned in Section 1, the physics of the Mott-Hubbard metal-insulator transition is of first order in the HM ($D_f/D_c = 1$), and hence accompanied by a hysteresis loop in the phase diagram. This hysteresis loop is obtained numerically as follows: increasing $U$ by taking a DMFT solution of a smaller $U$ as a starting point for the next DMFT iteration, yields a metallic solution up to a critical interaction $U_{c1}$. Above $U_{c1}$, the metallic (M) solution is no longer stable and the system becomes Mott-insulating (I) instead. Decreasing $U$ from here, yields an insulating solution down to a second critical interaction $U_{c2} < U_{c1}$. Hence, in the limit of the HM, where $c$ and $f$ fermions are equally mobile, there is a coexistence region of the M and the I phase for $U_{c2} < U < U_{c1}$. The Mott-Hubbard metal-insulator transition in the HM has been investigated thoroughly in the literature, among others for the semi-elliptic Bethe DOS [7,26]. In the FKM on the other hand no coexistence region is observed. The Mott-like metal-insulator transition occurs temperature-independent exactly at $U_c = D_c$ in the FKM, as is analytically known and well reviewed in reference [8], also see Figure 1.

Figure 2 shows the phase diagram $D_f/D_c$ vs. $U$ of the mass-imbalanced HM inbetween these two known limits at two inverse temperatures $\beta = 50$ and 100. The first order coexistence region has been determined in the same way as described above for the HM: the four green symbols in Figure 2 mark up to which point an M or I solution is found upon increasing or decreasing $U$. We observe a coexistence region and hence a first order transition in a wide range of mass imbalances. The coexistence region is increasing upon decreasing temperature to $\beta = 100$, and the critical point where the first order transition ends (green circle, $D_{crit}$) is moving towards the FKM limit $D_f/D_c = 0$. To obtain the phase diagram, we discriminate between M and I solution by means of the imaginary part of the self-energy $\Sigma_i(\omega_n)$.

Figure 3 shows this imaginary part of the self-energy for exemplary $U$ values at $\beta = 100$. In panel (a) the results for the HM are shown: specifically, one metallic (M, $U = 4.6$, blue) and one insulating solution (I, $U = 4.9$, orange) upon decreasing $U$ ($\rightarrow$), as well as one M ($U = 5.2$, cyan) and I solution ($U = 5.5$, red) upon increasing $U$ ($\leftarrow$). The insulating solution is characterized by a divergence $\Sigma_i(\omega_n) \rightarrow -\infty$ for $\omega_n \rightarrow 0$, and we take this as the criterion for discriminating M and I solutions in the phase diagram (Fig. 2).

Figure 3b displays the results for the FKM: analogously, one metallic solution ($U = 1.5 < U_c$, blue) and one insulating solution ($U = 2.5 > U_c$, red) are shown. Since there is no coexistence region in the FKM, we instead additionally show the solution for the unique and temperature-independent $U_c = 2$ (yellow).

Figures 3c and 3d display analogous phase points though now for the mass-imbalanced HM at a mass imbalance $D_f/D_c = 0.4$, which is inbetween the limiting cases of the HM (a) and FKM (b). The more mobile c fermions are shown in Figure 3c, and the less mobile f fermions in (d). The shift of the Mott-insulator transition compared to the HM is taken into account by adjusting the interaction strength to $U = 3.2$ ($\leftarrow$ M, blue), $U = 3.3$ ($\leftarrow$ I, orange), $U = 3.4$ ($\rightarrow$ M, cyan) and $U = 3.5$ ($\rightarrow$ I, red) in the two lower panels. We observe that the $c$ fermions
undergo a stronger renormalization than the already less mobile, and thus heavier, $f$ fermions. That is, in the metallic phase the effective mass enhancement

$$m^*/m = Z^{-1} = 1 - \partial \text{Im} \Sigma(i\omega_n)/(\partial i\omega_n)|_{\omega_n \to 0} \quad (2)$$

is stronger for the $c$ fermions. Nonetheless, the divergent $\text{Im} \Sigma(i\omega_n) \sim -1/(i\omega_n)$ behavior of the self-energy which indicates the insulating phase sets in at the same $U$ value. Overall both self-energies in (c, d) look similar as for the HM in (a) except for the smaller $\omega_n$ ($x$-axis) scale, which can be understood from the lower $U$ value of the Mott transition.

In Figure 4, we extrapolate the coexistence region which is shrinking with decreasing $D_f/D_c$ to $U_{c1} - U_{c2} = 0$. This marks the temperature-dependent critical point $D_{\text{crit}}(\beta)$ at which the first order transition ends, denoted by a green circle in Figure 4. At the lower temperature ($\beta = 100$) this critical point is already very close to the FKM limit $D_f/D_c = 0$, which together with the apparent temperature dependence suggests that indeed for zero temperature $D_{\text{crit}}(\beta = \infty) = 0$. In other words, the FKM appears to be the critical point of the mass-imbalanced HM at zero temperature.

The double occupancy in Figure 5 likewise shows the first order transition and hysteresis loop in $U$. In the Mott-insulating phase each site is essentially singly occupied. We see that the spectral function $\langle \hat{n}_c \hat{n}_f \rangle$ for different values of the mass imbalance $D_f/D_c$ at $\beta = 50$ (upper panel) and $\beta = 100$ (lower panel), showing the hysteresis loop of the first order transition upon increasing and decreasing $U$. In contrast to when approaching the metallic phase upon decreasing $U$, the higher kinetic energy leads to a strong increase in the number of doubly occupied sites. Only in the limit $U \to 0$ the uncorrelated double occupation $\langle \hat{n}_c \hat{n}_f \rangle = 1/4$ is eventually recovered. The figure shows again clearly that the coexistence region increases upon decreasing temperature (increasing $\beta$). On that ground the behavior of the mass-imbalanced HM is similar to the HM also regarding the double occupation.

Figure 6 shows the corresponding spectral function comparing the HM ($D_f/D_c = 1$) and the mass-imbalanced HM ($D_f/D_c = 0.8$ and 0.6), immediately before (a, c) and after (b, d) the transition $U_{c1}$ where the metallic solution ceases to exist. We see that the spectral functions are actually quite similar with a three-peak structure on the metallic side, consisting of a lower and upper Hubbard band and a central quasiparticle peak in-between. Immediately after the transition $U_{c1}$ there is a gap in the insulating phase. This is very different from the FKM in Figure 1 where we have two peaks which do not overlap any more for $U$ below the transition, as opposed by the overlap for $U$ above the transition. There is also no indication of a smooth crossover in Figure 6 from the HM behavior to that of the FKM. The major difference is that with reducing $D_f/D_c$ in Figure 6, the position of the upper (lower) Hubbard band shift.
The physics in Figure 6 of the mass-imbalanced HM seems to resemble that of the HM rather than that of the FKM. Also in Figure 4 we have seen that the first order transition of the HM survives a quite considerable mass imbalance, down to even smaller $D_f/D_c$ values at lower temperatures. We know on the other hand that there is no first order transition for the FKM. This poses the questions whether at zero temperature $D_{\text{crit}} = 0$, i.e., there is always a first order transition for $D_f > 0$? Is the FKM and its physics a singular point of the mass-imbalanced Hubbard model at zero temperature? Indeed the temperature dependence in Figure 7 shows the analysis of the quasiparticle renormalization $Z_f$ for both fermionic species $x = c$ and $f$ fermions in Figure 6. The height of the central resonance, on the other hand, is independent of $D_f$ for the $c$ fermions (note $D_c = 2$ is fixed), whereas it increases $\sim 1/D_f$ for the less mobile $f$ fermions as does the non-interacting DOS of the $f$ fermions.

We can validate this expectation numerically by estimating the width of the central resonance as $Z_\omega D_x$, where $Z_\omega$ is the quasiparticle renormalization as calculated from the self-energy through equation (2). If the width $Z_\omega D_x$ is to be the same for the $x = c, f$ fermions, the quasiparticle renormalization $Z_f$ needs to be larger than $D_f < D_c$. Indeed a first indications for this we have already seen in the smaller $f$ self-energy and hence larger $Z_f$ in Figure 3.

Figure 7 shows the analysis of the quasiparticle renormalized width $Z_\omega D_x$ for the two fermionic species $x$. Indeed we see that $Z_c D_c$ is the quasiparticle renormalization as the metal-insulator transition is approached, in agreement with our considerations above. In contrast, at $U = 0$ where $Z_c = 1$ the width is obviously very different. For the exemplary green line in Figure 7, we see the continuous evolution from a factor

\[ G_\omega^{-1}(\omega) = \omega + \mu - (D_x/2)^2 G_x(\omega) \equiv \omega + \mu - \Delta_x(\omega), \tag{3} \]

given by the interacting Green function $G_x(\omega)$ at frequency $\omega$ [7]. This can be understood as follows: if a fermion leaves the impurity with amplitude $D_x/2$ it propagates through the strongly correlated bath of the other sites given by $G_x(\omega)$ before returning to the impurity with amplitude $D_x/2$. The difference for the mass-imbalanced HM is now that each fermion species $x = c, f$ has an individual bath or hybridization function $\Delta_x(\omega)$.

On the metallic side, close to the metal-insulator transition we have seen a narrow central resonance in Figure 6, and we can map the Anderson impurity model onto a Kondo model with different baths. For a narrow resonance, we are in the Kondo regime and can apply the perturbative renormalization group also known as Anderson’s poor man scaling [33,34] for understanding the physics. For the renormalization of the Kondo coupling, the spectral weight at high energies, i.e., in the upper and lower Hubbard band does not matter and we can restrict ourselves to the central resonance [35].

Since the Kondo effect relies on spin-flip (i.e., $c$-$f$) scattering [34], it is not possible that the coupling to the bath for one species alone becomes large in the renormalization process whereas the other does not. The two fermionic species make the Kondo effect at essentially the same Kondo temperature and develop a Kondo resonance together. This also implies that the physical origin of the central resonance and its width is the same for $c$ and $f$ fermions in Figure 6. The height of the central resonance, on the other hand, is independent of $D_f$ for the $c$ fermions (note $D_c = 2$ is fixed), whereas it increases $\sim 1/D_f$ for the less mobile $f$ fermions as does the non-interacting DOS of the $f$ fermions.

We can validate this expectation numerically by estimating the width of the central resonance as $Z_\omega D_x$, where $Z_x$ is the quasiparticle renormalization as calculated from the self-energy through equation (2). If the width $Z_x D_x$ is to be the same for the $x = c, f$ fermions, the quasiparticle renormalization $Z_f$ needs to be larger than $D_f < D_c$. Indeed a first indications for this we have already seen in the smaller $f$ self-energy and hence larger $Z_f$ in Figure 3.

4 At least as long as these Hubbard bands are well enough separated from the central resonance.

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3 Albeit the resolution is not perfect because of the maximum entropy analytic continuation.
of 0.6 difference in width at $U = 0$ to the same width in the Kondo regime in the vicinity of the phase transition line $U_c$. The general tendencies agree with [14] where an (imperfect) balancing effect of the interaction on the effective hopping has been reported. On top of this, Figure 7 also shows that a perfect balancing effect is obtained when approaching the Mott-Hubbard transition.

The observation that $Z_c D_c \rightarrow Z_f D_f$ for $U \rightarrow U_{c1}$ also implies a simultaneous phase transition for both fermionic species, in agreement with our observation for the self-energy in Figure 3 and the phase diagram in Figure 2. This is in contrast to the multi-orbital HM for which an orbital-selective phase transition has been observed [15–20]. The striking difference is that for the multi-orbital HM we have two spin species for each orbital so that the Kondo effect can occur separately for each orbital which is not possible in our case of the mass-imbalanced HM.

Altogether, the physics of the mass-imbalanced HM for $D_f > 0$ rather resembles that of the HM than that of the FKM. Noteworthy, however, one needs ever lower temperatures with decreasing $D_f$ in order for the central resonance to develop since the Kondo temperature decreases exponentially. The similar physics to the HM further suggest the same first order metal-insulator transition. Indeed the temperature dependence of the critical exponents broken in the early days of DMFT [36–38] and eventually had to be decided numerically. In our case of the mass-imbalanced HM our numerical data strongly indicates that the phase transition already becomes first order as soon as there is a finite hopping of the $f$ fermions ($D_f > 0$).

5 Conclusion

We have analyzed the Mott-insulator transition of the mass-imbalanced Hubbard model within the paramagnetic phase. Our phase diagram, Figure 2, shows a first order phase transition in a wide range of mass imbalances $D_f/D_c$. With decreasing temperature the region of first order coexistence expands; and our results suggest that the mass-imbalanced Hubbard model always displays a first order metal-insulator transition at zero temperature as soon as a small, but finite, hopping of the less mobile $f$ fermions is switched on ($D_f > 0$).

For the FKM ($D_f = 0$), we have two bands along with a gap opening with increasing $U$ as soon as these two bands do not overlap any longer. If we switch on $f$ fermion hopping however ($D_f > 0$), a central resonance in this gap develops due to the Kondo effect. This stabilizes the metallic phase and shifts the metal-insulator transition in the phase diagram in Figure 2 towards larger $U$ values. This resonance and a three-peak structure can be seen in the spectral function, Figure 6. We find that the width of the central resonance is the same for the $c$ and $f$ fermions. This can be understood from the fact that the spin–flip (here $c-f$) scattering is crucial for the Kondo effect. Hence we have a joint Kondo temperature and width of the Kondo resonance for $c$ and $f$ fermions.

This is affirmed by an analysis of the quasiparticle renormalization factor $Z_c$ in Figure 7, which shows $Z_c D_c \rightarrow Z_f D_f$ when approaching the metal-insulator transition, i.e. when we are in the Kondo regime accompanied by a narrow central resonance. It further shows that the metal-insulator transition occurs simultaneously for both, $c$ and $f$, fermions in the mass-imbalanced Hubbard model. The Falicov-Kimball physics, where the $f$ fermions are insulating for any $U$ and the $c$ fermions for $U > D_c$, is a singular point of the phase diagram at zero temperature.

Altogether our results show that the physics of the mass-imbalanced Hubbard model in the paramagnetic phase resembles that of the Hubbard model. This is because of the equalizing power of the joint Kondo effect of the two fermionic species. This also agrees with the observation in [14] that both fermionic species are Fermi liquids below a coherence energy scale.

Regarding the antiferromagnetic phase we nonetheless expect a qualitatively different behavior: the mass imbalance breaks the $c-f$ O(3) rotational symmetry of the order parameter; and Monte-Carlo simulations [13] indeed indicate an Ising-type ordering. Hence we expect Ising-type critical exponents similar to what has recently been reported for the FKM [39], whereas we have a Heisenberg-type of ordering and associated critical exponents [40] for the Hubbard model.

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Author contribution statement

Marie-Therese Philipp performed the numerical simulations, prepared the figures and partly wrote the manuscript. Markus Wallerberger initiated the project, gave essential counseling regarding the computations and QMC algorithm. Patrik Gunacker performed the maximum entropic analytic continuation and helped in the writing process. Karsten Held guided the project, gave essential interpretations, and wrote a major part of the manuscript.

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