Multiband Dual Fermion Approach to Quantum Criticality in the Hubbard Honeycomb Lattice

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(Dated: October 24, 2017)

We study the Hubbard model on the honeycomb lattice in the vicinity of the quantum critical point by means of a multiband formulation of the Dual Fermion approach. Beyond the strong local correlations of the dynamical mean field, critical fluctuations on all length scales are included by means of a ladder diagram summation. Analysis of the susceptibility yields an estimate of the critical interaction strength of the quantum phase transition from a paramagnetic semimetal to an antiferromagnetic insulator, in good agreement to other numerical methods. We further estimate the crossover temperature to the renormalized classical regime. Our data imply that, at large interaction strengths, the Hubbard model on the honeycomb lattice behaves like a quantum nonlinear σ model, while being in a non-Fermi liquid state.

PACS numbers: 71.30.+h71.10.Fd, 71.10.-w,

I. INTRODUCTION

The Hubbard model is widely believed to capture some of the most exciting phenomena in strongly correlated electron systems, including unconventional superconductivity1, itinerant magnetism, non-Fermi-liquid behavior2 and quantum criticality. The nature of its ground state is determined decisively by the underlying lattice. Since the discovery of graphene3, the half-filled Hubbard model on the honeycomb lattice has been intensely studied with a variety of techniques, each having their respective advantages and limitations. They nevertheless agree concerning the existence of a quantum critical point at finite value of the interaction strength.

The application of projective quantum Monte Carlo to the ground state has raised speculations about the existence of a spin-liquid phase at zero temperature4. Later studies revealed that an extrapolation from sufficiently large lattice sizes causes the semimetal-insulator transition and the onset of an antiferromagnetically ordered ground state to coincide5,6. This leaves a vanishingly small window for the existence of a spin liquid.

Thus far the value of the critical Hubbard interaction $U_c$ for the quantum phase transition from the semimetal to the antiferromagnet has been calculated with a variety of methods, with results ranging from 3.5 to 5 (all values in units of the hopping t). The more recent works almost entirely find values close to 3.8. The introduction section of Ref. 7 provides a good overview over existing results, while here we only quote the more recent ones, that agree closely and that we consider the most accurate: Large scale projective quantum Monte Carlo (QMC)5 yields $U_c = 3.869 \pm 0.0013$, while the pinning-field QMC measurements used in Ref. 6 result in $U_c = 3.78 \pm 0.001$. The dynamical cluster approximation (DCA) gives $U_c = 3.69$ using up to 96 cluster sites8. Functional renormalization group investigations9,10 find $U_c = 3.8$, while a study based on the two-particle self-consistent (TPSC) method reports $U_c = 3.79 \pm 0.01$11.

In this paper, we address this problem by means of the Dual Fermion (DF) approach11. DF belongs to the recently developed important class of methods known as diagrammatic extensions of dynamical mean-field theory12. Their common feature is a perturbative expansion of the self-energy in terms of a dynamical vertex of the underlying the DMFT impurity problem. While the self-energy is approximate, correlations are included on all length scales. Notably, diagrammatic extensions have been shown to recover nonlocal correlation phenomena such as pseudogap formation13, formation of extended van Hove singularities14 and (quantum) criticality15 including non mean-field critical exponents16.

The reasons for applying DF to the Hubbard honeycomb lattice are twofold: firstly, we aim to provide an independent viewpoint on the physics of this model by a method that is quite different in spirit from the ones previously applied to the problem as mentioned above; secondly, we show that DF captures the physics of the quantum critical point and even yields a quantitative estimate of the critical interaction. To this end, we generalize the ladder DF approach (LDFA)13 to account for multiple atoms in the unit cell in a multiband extension. This allows us to numerically establish the connection between the large interaction limit of the Hubbard model on the honeycomb lattice and the renormalization group treatment of the quantum nonlinear σ model as in Ref. 17.

II. MODEL AND METHOD

We formulate the problem for two atoms in the unit cell adapted the honeycomb lattice, although the extension to an arbitrary number of atoms is straightforward. For each atom one in general has to solve an impurity problem, similarly to real-space DMFT (RDMFT)18. Here the two impurity problems are equivalent owing to the equivalence of two sublattices. In DMFT the inter-site self-energy is zero, whereas in DF it is included diagrammatically. In principle it is possible to start from a cluster formulation and to include diagrams beyond DCA19 or CDMFT20, which however breaks lattice symmetries artificially depending on the choice of the cluster problem (see Fig. 1).

For the Hubbard model on a lattice with multiple atoms per
is exactly mapped onto an equivalent one in terms of dual
is diagonal in sublattice space, \( \hat{\Delta} \), where the hybridization matrix of the impurity problem \( \hat{\Delta} \) action in terms of these as follows:

\[
S[c^\dagger c] = \sum_{\nu \kappa A B \sigma} c^\dagger_{\nu \kappa A \sigma} \left[(i\nu + \mu) \delta_{AB} - \hat{\epsilon}(\kappa)_{AB}\right] c_{\nu \kappa B \sigma} + \sum_{\omega, \tau, A} n_{\omega A \tau} n_{-\omega A \tau},
\]

(1)

where \( \nu \) (\( \omega \)) represents fermionic (bosonic) Matsubara frequencies and \( \kappa \) the lattice momentum, \( \hat{\Gamma} = 1/T \) is the inverse temperature and \( \mu \) the chemical potential. We assume that the Coulomb repulsion is restricted to on-site terms of strength \( U \). The lattice is divided into sublattices as shown in Fig. 2. The sum over sublattice indices \( A, B \) runs over all \( N \) atoms in the unit cell. Small Latin indices label the sites on the Bravais lattice (conjugate variables to the lattice momenta) and \( \sigma = \uparrow, \downarrow \) represents the spin projection. We generally drop spin indices on single-particle quantities as we only consider the SU(2) symmetric case. The dispersion \( \hat{\epsilon}(\kappa) \) is an \( N \times N \) matrix in sublattice indices. Its off-diagonal elements account for the hopping between sublattices. Here and in the following we indicate matrix-valued functions with a caret.

\[\hat{\Gamma}, \hat{\Delta}, \hat{\Delta}_{AB} = \hat{\Delta}_{A} \delta_{AB}\]

where dual quantities are marked by a tilde and Greek letters denote compound indices, \( \alpha = \{\nu \sigma\} \). Since the hybridization and Coulomb interaction are local, the impurity vertex is diagonal in sublattice indices as well, \( \gamma_{ABCD} = \gamma^{\alpha\beta\gamma\delta} \delta_{AB} \delta_{CD} \), and we abbreviate \( \gamma^A \equiv \gamma^{\alpha\beta\gamma\delta} \). Details of this transformation can be found in the Appendix.

The dual fermions can be thought of as mediating the coupling between the impurities on different sites of the Bravais lattice. The underlying idea is that a perturbative solution of this problem in terms of the bare dual Green function \( \hat{\Gamma}^{(0)}_{\nu} \) and interaction \( V[f^*, f] \) contains the correlated non-perturbative local physics from the start (at zeroth order).

While for graphene the sublattices are equivalent, symmetry breaking between sublattices can be induced locally in our approach for example through a sublattice-dependent chemical potential or Coulomb interaction, or via the dispersion matrix (consider a bilayer honeycomb lattice with layer-dependent hopping amplitudes).

\[S[f^*, f] = -\sum_{\nu \kappa A B \sigma} f^{\dagger \nu} \gamma^{\nu} \sigma f_{\nu \kappa A \sigma} - \sum_{\nu} \sum_{\alpha \beta \gamma \delta} \gamma^{\nu} \sigma_{\alpha \beta \gamma \delta} f^{\dagger \nu} \sigma f_{\nu \kappa A \sigma}, \]

(2)

A. Dual Fermions

We briefly outline the derivation and discuss the structure of the DF approach specific to the multiband case. Further details on the derivation and the approach can be found in the Appendix and Ref. 12. We first introduce an Anderson impurity problem for each sublattice and express the lattice action in terms of these as follows:

\[S[c^\dagger c] = \sum_{\nu} S_{\text{imp}}[c^\dagger_{\nu A \sigma}, c_{\nu A \sigma}] - \sum_{\nu \kappa A B \sigma} c^\dagger_{\nu \kappa A \sigma} \left[\hat{\Delta}_{\nu} - \hat{\epsilon}(\kappa)_{AB}\right] c_{\nu \kappa B \sigma}, \]

(2)

where the hybridization matrix of the impurity problem \( \hat{\Delta} \) is diagonal in sublattice space, \( \Delta_{AB} = \Delta_{A} \delta_{AB} \). This action is exactly mapped onto an equivalent one in terms of dual

\[\hat{\Gamma}_{\nu \nu^\prime \Omega q} = \hat{\Gamma}_{\nu \nu^\prime \Omega q} - \frac{1}{\hat{\Gamma}_{\nu \nu^\prime \Omega q}} \sum_{\nu^\prime} \hat{\Gamma}_{\nu \nu^\prime \Omega q} \hat{\Gamma}_{\nu^\prime \nu^\prime \Omega q} \hat{\Gamma}_{\nu^\prime \nu \Omega q}, \]

(4)

B. Ladder approximation

To describe the physics in the vicinity of the quantum critical point, we need an approximation that includes long-range fluctuations. Physically we expect (magnetic) particle-hole fluctuations to dominate. The corresponding diagrams are depicted in Fig. 3. The approximation is akin to the fluctuating exchange approximation (FLEX), albeit in dual space. The Bethe-Salpeter equation (BSE) is given by (all quantities such as Green’s functions in this section are dual by default)

\[\hat{\Gamma}_{\nu \nu^\prime \Omega q} \]
where \( \hat{\Gamma}^- \) is the dual renormalized lattice vertex and \( \hat{\chi}^0 \) the reducible impurity vertex in spin and charge channels \( c = \text{sp, ch} \). The latter vertex approximates the dual irreducible vertex of the lattice. The charge and spin components of the vertices are given by \( \Gamma^{\text{sp(ch)}} = \Gamma^{++\pm\pm} + \Gamma^{\pm\pm\pm\pm} \), \( \hat{\chi}^{(0)} \) is the dual particle-hole bubble,

\[
\hat{\chi}^{(0)AB}_{\nu\nu_0q} = \frac{1}{N} \sum_k \hat{\chi}^{AB}_{\nu+\omega_0+q} g_{\nu_0k},
\]

where we have used the shorthand notation \( \hat{\chi}^A \equiv \hat{\chi}^{ABB} \). Note that only terms of this form contribute because the local vertex is diagonal in the sublattice indices.

The matrix structure of the quantities in the BSE in sublattice space is as follows:

\[
\hat{\Gamma}^-_{\nu\nu_0q} = \begin{pmatrix} \Gamma^{AA}_{\nu\nu_0q} & \Gamma^{AB}_{\nu\nu_0q} \\ \Gamma^{BA}_{\nu\nu_0q} & \Gamma^{BB}_{\nu\nu_0q} \end{pmatrix}, \\
\hat{\chi}^{(0)}_{\nu\nu_0q} = \begin{pmatrix} \chi^{(0)AA}_{\nu\nu_0q} & \chi^{(0)AB}_{\nu\nu_0q} \\ \chi^{(0)BA}_{\nu\nu_0q} & \chi^{(0)BB}_{\nu\nu_0q} \end{pmatrix}, \\
\hat{\gamma}_{\nu\nu_0} = \begin{pmatrix} \gamma^{AA}_{\nu\nu_0} & 0 \\ 0 & \gamma^{BB}_{\nu\nu_0} \end{pmatrix}.
\]

Note that the off-diagonal components of the lattice vertex stem solely from the bubble, which mixes the sublattice components. The solution of the BSE is obtained by inverting \( \hat{\Gamma}^{-1} = [\hat{\Gamma}^+ + \hat{\chi}^{(0)}]^{-1} \), for each channel and each value of the bosonic frequency \( \omega \) up to the cutoff. Correspondingly the matrices should be viewed as matrices in a combined frequency and sublattice index.

From the renormalized two-particle vertex we obtain the self-energy in the ladder approximation by means of the dual version of the Schwinger-Dyson equation (SDE). It is depicted in Fig. 3 and reads

\[
\hat{\Gamma}_{\nu\nu_0} = -\frac{T}{N} \sum_{v'\omega_0q} \gamma^{AA}_{\nu'v'\omega_0} \hat{\chi}^{AB}_{\nu\nu_0q} \left[ 2 \Gamma^{BB}_{\nu'v'\omega_0} - \gamma^{BB}_{\nu\nu_0} \delta_{BC} \right],
\]

\[
\hat{\gamma}_{\nu\nu_0} = \frac{T^2}{N^2} \sum_{v'\omega_0q} \gamma^{AA}_{\nu'v'\omega_0} \hat{\chi}^{(0)AB}_{\nu\nu_0q} \left[ 2 \Gamma^{BB}_{\nu'v'\omega_0} - \gamma^{BB}_{\nu\nu_0} \delta_{BC} \right],
\]

The factor 3/2 stems from the three-fold degeneracy of the spin-1 bosonic excitations in the spin channel.

C. Calculation procedure

The numerical calculation proceeds as follows. We first perform DMFT iterations to obtain the starting point of our perturbation theory. Since DMFT corresponds to non-interacting dual fermions, we can achieve this by imposing a self-consistency condition on the bare local dual Green’s function,

\[
\sum_k \hat{g}^{AA}_{\nu k} = 0.
\]

The bare dual Green’s function can be written \( g^{(0)}_{\nu k} = \hat{g}^{\text{DMFT}}_{\nu k} - \hat{\gamma}_{\nu k} \). Eq. (8) is thus equivalent to the self-consistency condition in real-space DMFT when no diagrams are taken into account. Our results for the honeycomb lattice can therefore be interpreted as diagrammatic corrections to the DMFT results of Ref. 21. Once converged, we compute the vertex of the impurity model(s) and evaluate the self-energy according to Eqs. (4) and (7). The Green’s function is computed from the dual Dyson equation

\[
\hat{G} = \left( \hat{\gamma} + \hat{\chi} \right)^{-1} \left( \hat{\gamma} + \hat{\Delta} - \hat{\gamma} \right)^{-1}.
\]

The BSE, SDE and Dyson’s equation form a nonlinear set of equations which we solve self-consistently. We then update the impurity hybridization with the goal to fulfill the self-consistency condition (8) for the full dual Green’s function.

Finally, after convergence, the lattice Green’s function is readily obtained via

\[
\hat{G} = \left[ \left( \hat{\gamma} + \hat{\chi} \right)^{-1} + \hat{\Delta} - \hat{\gamma} \right]^{-1}.
\]

To evaluate the generalized susceptibility tensor we first transform the renormalized dual lattice vertex to the corresponding physical lattice vertex using Eq. (34). The generalized susceptibility tensor and the lattice vertex are related via

\[
\hat{\chi}^{AB}_{\omega_0} = -\frac{T}{N} \sum_{v'\omega_0q} \Gamma^{AA}_{v'\omega_0} \hat{\chi}^{AB}_{v'\omega_0q} \left[ 2 \Gamma^{BB}_{v'\omega_0} - \gamma^{BB}_{v\omega_0} \delta_{BC} \right]
\]

\[
+ \frac{T^2}{N^2} \sum_{v'\omega_0q} \Gamma^{AA}_{v'\omega_0} \chi^{(0)AB}_{v\nu_0q} \left[ 2 \Gamma^{BB}_{v'\omega_0} - \gamma^{BB}_{v\omega_0} \delta_{BC} \right],
\]

(11)
The generalized susceptibility facilitates the analysis of phase transitions in multiband systems, since in general the order parameter is unknown and may have a complicated structure. The order parameter for multiband systems can be deduced from the leading eigenvalue of the generalized susceptibility tensor as demonstrated in Ref. 22.

III. RESULTS

We now turn to the Hubbard model on the honeycomb lattice. The Hamiltonian is given by

$$H = \sum_{kAB} \epsilon_k \hat{c}_k^\dagger \hat{c}_k^{AB} + U \sum_T (n_{A\uparrow} n_{A\downarrow} + n_{B\uparrow} n_{B\downarrow}),$$

$$\hat{\epsilon}_k = \begin{pmatrix} \epsilon(k) & -t f(k) \\ -t f^*(k) & 0 \end{pmatrix},$$

$$f(k) = e^{-i\gamma k_y} + 2e^{i\pi k_x} \cos \left( \frac{a}{2} k_z \right).$$

We use the nearest-neighbor hopping amplitude $t$ as the energy unit and set the lattice constant $a = 1$. The impurity problem is solved using a hybridization expansion quantum Monte Carlo algorithm with improved estimators for the vertex function. We employ a finite cutoff of the Matsubara frequencies of the impurity Green’s function $g_\nu$ and two-particle vertex $\gamma_{\nu\nu'\omega}$ with $|\nu| \leq (2n_1 + 1)\pi T$ as well as $|\nu|, |\nu'| \leq 2n_2 + 1\pi T$ and $|\omega| \leq 2m\pi T$. We choose $n_1 = 128$ and $n_2 = 64$. The single-particle Green’s function is already well in its tail behavior described by the first few powers of $1/(iv_n)$ for this value of $n_1$. We further checked that changes in the dual self-energy are negligible when the cutoff $n_2$ is increased. In order to determine the quantum critical point (QCP) the cutoff $m$ for the bosonic frequency and the lattice size are varied (see below). We checked numerically that in the weak coupling limit $U \leq 1$ our implementation is equal to FLEX.

A. Quantum Critical Point

We investigate the model in the vicinity of the critical point. As $U$ is increased beyond $U_c$, the ground state changes from a semimetal to an antiferromagnet. In order to determine $U_c$, we analyze the leading eigenvalue of the matrix $M = T \gamma \hat{\chi}$, where $\gamma$ and $\hat{\chi}$ are defined in (6). Matrices with leading eigenvalues of $\lambda = 1$ are outside of the convergence radius of the geometric series and indicate the divergence of the ladder series due to a phase transition. Hence $1 - \lambda$ is a useful measure for the criticality of the system.

At half-filling and large $U$ the Hubbard model can be mapped to an antiferromagnetic Heisenberg model, which can be described by a quantum nonlinear $\sigma$ model in two dimensions in the long-wavelength, low-temperature limit. In the renormalized classical regime the correlation length scales as $\xi^{-1} \propto 1/\beta \exp(-2\pi \rho \beta)$, where $\rho$ is the ground state spin stiffness. At the quantum critical point $\rho = 0$ and therefore $\xi^{-1} \propto 1/\beta^{17}$. The log scale plots on the left hand side of Fig. 4 reveal that $1 - \lambda$ exhibits the same behavior as $\xi^{-1}$.
since \((1 - \lambda)\beta\) is a constant close to \(U = U_c\), while for \(U > U_c\) \((1 - \lambda)\beta\) decays exponentially. Note that the rate of decay increases as \(U\) increases. In order to estimate the crossover temperature \(T_c\), where the system enters the renormalized classical regime, the correlation length \(\xi\) has been equated to the thermal wavelength of spin waves in Ref. 17 or free electrons in Ref. 7. Here, using that \(1 - \lambda\) is proportional to the inverse correlation length, we can estimate \(T_c\) by requiring \((1 - \lambda)/T_c = C\), where the constant \(C\) is chosen such that the exponential decay of \(1 - \lambda\) is evident from the data for \(U > U_c\) and the system has already entered the renormalized classical regime. In particular, we choose \(C = 0.1\) and 0.05 (see red and blue lines on left hand side of Fig. 4). Power-law fits to the data \(T_c \propto (U/U_c - 1)^\nu\) yield good agreement with other numerical methods for the critical coupling \(U_c\). We find \(\nu = 0.7 - 0.8\) which is close to the value \(\nu = 0.7\) for the Heisenberg model in 2+1 dimensions\(^{17}\).

Analysis of the generalized susceptibility tensor confirms that the system has a tendency to AFM order. In Fig. 5 we plot the inverse of the AFM susceptibility, which is given by \(\langle (S_A^z - S_B^z)^2 \rangle_{\text{eq}} = 0\), with \(S_A^z = n_{A\uparrow} - n_{A\downarrow}\) and \(A \neq B\), for different lattice sizes and values of \(U\). The data shows no tendency to AFM ordering at finite temperature, as required by the Mermin-Wagner theorem. While the AFM ground state is expected to be dependent on lattice size\(^{15}\), this is not the case for a semimetallic ground state. As \(U\) is decreased starting from \(U > U_c\), we can see that the susceptibility and leading eigenvalue become less size dependent and less divergent as the ground state changes from AFM to a semimetal. We defining the lower bound for the critical coupling \(U_{c1}\) as the value of \(U\) for which the according curves are virtually on top of one another, and the upper bound \(U_{c2}\) as the value for which the size dependence is evident and \((1 - \lambda)\beta\) is a straight line in the log scale plot. We take the estimate for \(U_c\) to be their average, ranging from 3.6 to 3.8 in units of the hopping for \(N_W = 1\) to \(N_W = 16\) respectively, which gives good agreement with \(U_c\) drawn from the fits in Fig. 4. For practical numerical purposes it is important to note that using a single bosonic frequency is sufficient to get a good estimate of \(U_c\), while for \(N_W = 16\) we had to go to lattice sizes of 144 x 144 to recover a straight line in the log scale plot for \(U > U_c\). Note that as one increases the number of bosonic frequencies accounted for in the LDFA simulations, the value for the critical coupling \(U_c\) is shifted to larger values, as more long-ranged spin fluctuations destroy the AFM order.

**B. Semimetal Insulator Transition**

Being restricted to finite temperatures, we obtain information about the conducting properties of the ground state using polynomial extrapolations of the quantity

\[
Z_k(T) = \left[1 - \frac{\text{Im} \Sigma_k(\pi T)}{\pi T} \right]^{-1}
\]

to the limit \(T \to 0\), which equals the quasiparticle renormalization factor\(^8\). As the self-energy in our problem is matrix-valued, we consider the trace of Eq. (13).
The corresponding data, again for different number of bosonic frequencies, is shown in Fig. 6. While projective QMC calculations with size extrapolation\(^5,6\) indicate that the interaction strengths marking the onset of the AFM phase \((U_c)\) and the opening of the single-particle gap \((U_{SMIT})\) coincide, extrapolation of our data instead gives \(U_c - U_{SMIT} \approx 0.3t\), regardless of the number of bosonic frequencies. Therefore our data contains no hint towards the existence of a spin liquid phase. Due to the extrapolation over a rather wide temperature range it is difficult to draw final conclusions whether \(U_c\) is actually different from \(U_{SMIT}\).

Looking for a possible semimetal insulator transition (SMIT) at finite temperature we perform analytical continuation of the self-energy using Padé approximants. We compute the quasi-particle renormalization factor from

\[
Z = \left[ 1 - \frac{\partial \text{Re} \Sigma_{k,\omega}}{\partial \omega} \right]_{k=k_F,\omega=0}^{-1},
\]

where \(\omega\) labels real frequencies. Surprisingly, we find that \(Z\) increases with \(U\) above a certain threshold as depicted in panels a) and b) of Fig. 7. The figure illustrates that this behavior appears to be robust, occurring for different temperatures and number of bosonic frequencies alike. In panel c) we show the result of the analytically continued self-energy at \(U = 3.8\) and \(T = 1/30\). The main panel shows the imaginary part, while the real part is shown in the inset. The distinct kink in \(\text{Im} \Sigma\) and the inflection point in \(\text{Re} \Sigma\) around \(\omega = 0\) indicate that the system leaves the Fermi-liquid (FL) regime at finite temperature as \(U\) is increased. The inset in panel d) of Fig. 7 shows a doubly logarithmic plot of the imaginary part of the diagonal of the self-energy at the Dirac point for interactions \(U/t = 2 - 3.8\) at the same temperature on the Matsubara axis, implying a power-law behavior. Furthermore the main panel d) shows the result of power law fits according to \(\text{Im} \Sigma \propto (i\nu_n)^\alpha\) to the data against the interaction. As the value of \(U\) increases the exponent of the power-law \(\alpha\) decreases to values as low as \(\alpha \approx 0.5\), which clearly deviates from the Fermi-liquid value \(\alpha = 1\). In Refs. 24 and 26 the phase boundary of the transition to a frozen moment phase has been defined by the requirement that the exponent be \(\alpha = 0.5\). Note that the self-energy on the real frequency axis in panel c) bears similarity to the results shown in Ref. 24. However we were not able to establish the existence of a frozen moment phase from the susceptibility data. The onset of the non Fermi-liquid behavior is still remarkably coincident with the critical coupling of the AFM transition. The value of \(\alpha\) suggests that for \(U > U_c\) the system is in a non-Fermi liquid state at finite temperature.

IV. CONCLUSIONS

In summary, we have presented a multiband extension of the Dual Fermion approach and applied it to the half-filled Hubbard model on the honeycomb lattice. We have found clear signs of the quantum phase transition from a paramagnetic semimetal to an AFM insulator in our data, in particular in the size dependence and divergence of the leading eigenvalue of the Bethe-Salpeter equation as well as in the self-energy. Analysis of the leading eigenvalue has further enabled us to compute the crossover temperature \(T_c\) to the renormalized classical regime and connect the strong-coupling limit to
the quantum nonlinear \( \sigma \) model. The numerical value where AFM ordering sets in at \( U_c \approx 3.6 - 3.8 \), is in good agreement with a variety of other numerical methods. Analysis of the self-energy suggests that for \( U > U_c \) the system behaves like a non-Fermi liquid at finite temperature.

V. ACKNOWLEDGEMENTS

The authors thank Eugene Kogan, Alexey N. Rubtsov, Mikhail I. Katsnelson and Guy Cohen for fruitful discussions. This work has been supported by Deutsche Forschungsgemeinschaft through the excellence cluster “The Hamburg Centre for Ultrafast Imaging - Structure, Dynamics and Control of Matter at the Atomic Scale” and from the European Graphene Flagship. Computational resources were provided by the HLRN-Cluster under Project No. lhnp00030.

MULTIBAND DUAL FERMION APPROACH

The derivation of the multiband approach is a special case of the general matrix formulation for multi-orbital problems and can be found in Refs. 28 and 29. We provide an outline of the derivation of the multiband formalism for local Coulomb interaction for the paper to be self-contained.

The partition function and action for the multiband Hubbard model are given by

\[
\mathcal{Z} = \int \mathcal{D}[\psi^*, \psi] \exp(-S[\psi^*, \psi])
\]

\[
S[\psi^*, \psi] = -\sum_{\mathbf{k} \mathbf{k}^\prime \sigma} \psi^*_\mathbf{k} \mathbf{\alpha} \left[ (\mathbf{i} \nu + \mu) \hat{\Delta}_\mathbf{k} \hat{\Delta} - \hat{\mathbf{e}}(\mathbf{k})_{\mathbf{\alpha} \mathbf{\alpha}^\prime} \right] \psi_{\mathbf{k}' \mathbf{\alpha}^\prime} + U \sum_{\mathbf{i} \mathbf{\alpha} \mathbf{\alpha}^\prime} n_{\mathbf{i} \mathbf{\alpha}} n_{\mathbf{i} \mathbf{\alpha}^\prime}.
\]

The labeling conventions are the same as in the main text. The main step is to express the lattice action in terms of the impurity action \( S_{\text{imp}} \) by adding and subtracting an arbitrary, frequency dependent hybridization matrix \( \hat{\Delta}_\mathbf{k} \) to the action Eq. (1),

\[
S[\psi^*, \psi] = \sum_{\mathbf{i} \mathbf{\sigma}} S_{\text{imp}}[\psi^*_\mathbf{i} \mathbf{\sigma} \psi_{\mathbf{i} \mathbf{\sigma}}] - \sum_{\mathbf{v} \mathbf{k} \mathbf{k}^\prime \mathbf{\sigma} \sigma^\prime} c^*_\mathbf{v} \mathbf{k} \mathbf{\alpha} \left[ \hat{\Delta}_\mathbf{k} - \hat{\mathbf{e}}(\mathbf{k})_{\mathbf{\alpha} \mathbf{\alpha}^\prime} \right] c_{\mathbf{v} \mathbf{k}' \mathbf{\alpha}^\prime},
\]

where \( S_{\text{imp}}[\psi^*_\mathbf{i} \mathbf{\sigma} \psi_{\mathbf{i} \mathbf{\sigma}}] \) is the action of a single impurity Anderson model on site \( \mathbf{i} \) and sublattice \( \mathbf{A} \):

\[
S_{\text{imp}}[\psi^*, \psi] = -\sum_{\mathbf{v} \mathbf{\sigma}} c^*_\mathbf{v} \mathbf{\sigma} \left[ (\mathbf{i} \nu + \mu) \mathbf{1} - \hat{\Delta}_\mathbf{k} \right]_{\mathbf{A} \mathbf{B}} c_{\mathbf{v} \mathbf{\sigma}} + U \sum_{\mathbf{\alpha}} n_{\mathbf{A} \mathbf{\alpha}} n_{\mathbf{B} \mathbf{\alpha}^\prime}.
\]

Dual fermions, represented by Grassmann fields \( f \) and \( f^* \), are introduced using a Hubbard-Stratonovich transformation.
(HST) to the second term in Eq. (17) according to
\[ \exp(c_i^* \hat{b}_j + \hat{a}_j^* c_i) = \frac{1}{\det \mathcal{D}[f^*, f]} \mathcal{D}[f^*, f] \exp(-f_i^* a_j + f_j^* b_i + c_i^* b_j f_j) \]
(19)
where \( g \) is the impurity Green’s function corresponding to the impurity problem defined by Eq. (18) and \( \hat{a} \) and \( \hat{b} \) are in principle arbitrary matrices which are set to above expressions for convenience. Thus one arrives at
\[ S[c^*, c, f^*, f] = \sum_i S_{\text{site}}[c_i^*, c_i] + \sum_{\nu, k, A, B, \sigma} f_{vkA\sigma} \left[ \hat{g}^{-1} (\hat{\Delta}_v - \hat{\epsilon}_k) \right]^{-1} f_{vkB \sigma} \]
(20)
\[ S_{\text{site}}[c_i^*, c_i] = S_{\text{imp}}[c_i^*, c_i] + \sum_{\nu, j, A, B, \sigma} f_{vjiA\sigma} c_{vijB\sigma} + c_{vijA\sigma} \left[ \hat{g}_v \right]^{-1} f_{vijB\sigma}. \]
(21)
\[ S_{\text{site}}[c_i^*, c_i] = S_{\text{imp}}[c_i^*, c_i] + \sum_{\nu, j, A, B, \sigma} f_{vjiA\sigma} c_{vijB\sigma} + c_{vijA\sigma} \left[ \hat{g}_v \right]^{-1} f_{vijB\sigma}. \]
(22)
In this form the lattice fermions, represented by \( c \) and \( c^* \), from different sites are decoupled and can be formally integrated out, as outlined below. Thereafter one is left with an action that is entirely formulated in terms of dual fermions
\[ \tilde{\mathcal{S}}[f^*, f] = -\sum_{\nu, A, B, \sigma} f_{vkA\sigma} \left[ \tilde{G}_{vkAB} \right]^{-1} f_{vkB \sigma} + \sum_i V[f_i^*, f_i], \]
(23)
where \( \tilde{G}_{vkAB} \) is the bare propagator for dual fermions and the third line defines the dual Green’s function. The dual partition function is given by \( \mathcal{Z} = \mathcal{Z}/\det \left[ \hat{\Delta} - \hat{\epsilon} \right] \cdot \hat{\Delta}^{-1} \). The second term in Eq. (24) gathers all terms that are of higher order in \( f^* \) and \( f \) than the bilinear term. It defines the interaction \( V[f^*, f] \) between dual fermions and results from expanding \( \exp(-S_{\text{site}}) \) in powers of \( f^* \) and \( f \). Because the partition function contains \( \exp(-S_{\text{imp}}) \), integrating out the lattice fermions produces (connected) correlation relations of the impurity. The dual interaction is correspondingly given by
\[ V[f^*, f] = -\frac{1}{4} \chi_{\text{imp}}^{\text{imp}} \lambda^{\text{imp}} \lambda^{\text{imp}} \]
(24)
where all degrees of freedom are merged into a compound index \( \alpha = \{ \nu, \sigma \} \). Repeated indices are summed over by convention. \( \gamma \) is the reducible two-particle impurity vertex. \( \chi^{(0)}_{\text{imp}} \) is the two-particle Green’s function of the impurity and \( \chi^{(0)}_{\text{imp}} \) is its disconnected part.

In order to compute observables of the original system consisting of lattice fermions \( c^* \) and \( c \), dual quantities have to be transformed after convergence of the perturbation series. In order to find the proper transformation consider the equality
\[ \mathcal{Z} = \int \mathcal{D}[c^*, c] \exp(-S[c^*, c]) \]
(25)
\[ = \mathcal{Z}_f \int \mathcal{D}[c^*, c, f^*, f] \exp(-S[c^*, c, f^*, f]), \]
(26)
which follows from the HST Eqs. (19)-(20) and \( \mathcal{Z}_f \) is the impurity located at site \( i \) on sublattice \( A \). Taking the functional derivative of Eq. (31) with respect to the one-particle Hamiltonian yields an identity relating the Green’s function of dual and lattice fermions
\[ \hat{G} = \left( \hat{\Delta} + \hat{\epsilon} \right)^{-1}. \]
(27)
Taking the according second derivatives yields a corresponding relation between two-particle Green’s functions, which in turn can be used to derive a relation between the full two-particle vertices of dual and lattice fermions
\[ \Gamma_{\alpha\beta\gamma\delta} = L_{\alpha\alpha'} L_{\gamma\gamma'} \lambda_{\alpha'\beta'\gamma'\delta'} R_{\beta'\beta} R_{\gamma'\gamma}, \]
(28)
\[ \hat{R} = \hat{g}^{-1} \hat{\Delta}^{-1} \hat{g}^{-1}, \]
(29)
\[ \hat{L} = \hat{g}^{-1} \hat{\Delta}^{-1} \hat{g}^{-1}. \]
(30)
