Local magnetic moment formation and Kondo screening in the half filled two dimensional single band Hubbard model

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We study formation of local magnetic moments in strongly correlated Hubbard model within dynamical mean field theory and associate peculiarities of temperature dependence of local charge $\chi_c$ and spin $\chi_s$ susceptibilities with different stages of local moment formation. Local maximum of temperature dependence of the charge susceptibility $\chi_c$ is associated with beginning of local magnetic moments formation, while the minimum of the susceptibility $\chi_s$ and double occupation, as well as low temperature boundary of the plateau of effective local magnetic moment $\mu_{\text{eff}} = T \chi_s$ temperature dependence are connected with full formation of local moments. We also obtain interaction dependence of the Kondo temperature $T_K$, which is compared to the fingerprint criterion of Phys. Rev. Lett. 126, 056403 (2021). Near the Mott transition the two criteria coincide, while further away from Mott transition the fingerprint criterion somewhat overestimates Kondo temperature. The relation of the observed features to the behavior of eigenvectors/eigenvalues of fermionic frequency-resolved charge susceptibility and divergences of irreducible vertices is discussed.

Localization of electrons in solids by correlation (interaction) effects yields formation of local magnetic moments, which are crucial for explaining observable magnetic properties of some of the existing materials and predicting new magnetic materials. Typical examples of importance of local magnetic moments include some aspects of the physical properties of high temperature superconductors in the underdoped regime [1, 2], modern explanation of ferromagnetism of transition metals, see, e.g., Refs. [3–7], as well as magnetic properties of iron pnictide superconductors [8, 9]. Local magnetic moments in the above mentioned substances appear due to electronic correlations in the proximity to the (orbital selective) interaction-induced Mott metal insulator transition (see, e.g., discussion in Refs. [10–12]) and/or due to Hund exchange interaction [3, 8, 13, 14].

Although the concept of metal-insulator transition was introduced by Mott in 1949 [15], quantitative studies of Mott transition became possible with the discovery of dynamical mean-field theory (DMFT) [16]. Originally, the Mott transition was described mainly on the basis of single-particle properties, e.g. spectral functions, densities of states etc. The three-peak structure of the density of states near Mott transition reflects coexistence of localized electrons (corresponding to the states in the Hubbard subbands) with itinerant degrees of freedom, described by the quasiparticle peak (see, e.g., Refs. [12, 16]). The developments of the non-local diagrammatic extensions of DMFT [17] yielded a new insight on the non-perturbative aspects of Mott transition via studying the divergences of the two-particle irreducible vertices [18–24]. These divergences were interpreted as the precursors of local moment formation [22, 25]. The formation of local magnetic moments was also recently discussed within non-local extensions of dynamical mean field theory in Ref. [26].

In the presence of conduction (itinerant) electrons (i.e. on the metallic side of Mott transition) the local moments are screened below certain characteristic (Kondo) temperature. In contrast to the standard Kondo effect, in strongly correlated substances the role of magnetic impurities is played by naturally occurring local magnetic moments and the same electrons participate in formation of local moments and their screening. This reflects the dual role of d-electrons, which was first discussed for transition metals by Vonsovskii [27] and more recently emphasized for pnictides [28–31]. Although the presence of characteristic (Kondo) temperature near Mott transition, below which almost formed local moments are screened by itinerant electrons, was emphasized in the early time of DMFT studies [32], the properties of Kondo screening near Mott transition were not intensively studied.

The Kondo temperature of local magnetic moments in strongly correlated systems can be extracted from comparison of the local spin susceptibility to that for the Kondo model [33, 34]. This approach was applied to extract Kondo temperature of Hund metals [5, 7, 35–39], as well as for description of Kondo screening in the Anderson impurity model [22, 25] and Hubbard model in the vicinity of Mott transition [36]. Therefore, it provides a unified view on the Kondo screening in strongly correlated substances.

We note that while the single impurity Kondo model can be considered as an effective low-energy model for the Anderson impurity model, its applicability for describing screening in lattice models, such as Hubbard model, is not a priori clear. On the other hand, due to reduction of the lattice problem to the impurity problem by DMFT, one can hope that at least within this theory the Kondo model is an appropriate effective low energy model for lattice problems too.

Recently, the two-particle criterion for the Kondo temperature in terms of frequency-dependent charge susceptibility was formulated for the Anderson impurity model in Ref. [25]. It was suggested that this criterion also applies to the Hubbard model in the vicinity of Mott transi-
tion. The generalization of this criterion for multi-orbital systems and fillings away from half filling is however not obvious. Somewhat different criterion of local moment formation was also proposed in Ref. [26].

In the present paper we consider the formation of local magnetic moments in single-band strongly correlated system, and study their screening properties on the verge of Mott metal-insulator transition. We use dynamical mean-field theory and study various local charge- and spin responses (susceptibility) to provide a unified view on the local magnetic moment formation in the considered model.

In particular, we address the following topics: (i) interaction dependence of the temperatures of beginning and full formation of local magnetic moments, as well as their screening (Kondo) temperature, and (ii) connection of Kondo screening to peculiarities of static charge susceptibility and double occupancy, the characteristic temperature scales of these quantities and their relation to Kondo temperature.

Model and method. We consider half filled Hubbard model on the square lattice

$$H = -t \sum_{\langle i,j \rangle, \sigma} c_{i\sigma}^\dagger c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow},$$

and use half band width $D = 4t = 1$ as the unit of energy.

Due to the assumption of locality of the self-energy, the DMFT [16] is a convenient tool to study formation and screening of local magnetic moments, which can be directly traced at the impurity site. To trace the formation of local moments we calculate in the self-consistent solution of DMFT the local spin susceptibility

$$\chi_s(i\omega_n) = \int_0^\beta \langle S^z(\tau)S^z(0) \rangle \exp(i\omega_n \tau) d\tau,$$

(Boltzmann’s constant is put to unity), $\omega_n = 2\pi nT$ are the bosonic Matsubara frequencies. We also consider local static charge susceptibility (local charge compressibility) $dn/d\mu = \chi_c(T)$, where the change of the chemical potential $d\mu$ acts only at the impurity site,

$$\chi_c(T) = \int_0^\beta \left( \langle n(\tau)n(0) \rangle - \langle n(0) \rangle^2 \right) d\tau = \sum_{\nu \nu'} \chi_c^{\nu \nu'}(T),$$

and use two- and single particle impurity Green’s functions (see Supplemental Material [40]).

For computations, we use the continuous time quantum Monte Carlo (CT-QMC) impurity solver, implemented in the iQIST software package [42]. At strong coupling and low temperatures near Mott transition we use numerical renormalization group (NRG) approach [43] within TRIQS-NRG Lyubilyana interface package [44] for calculation of correlation functions.

Results. We consider first the static local spin susceptibility $\chi_s(0)$, see Fig. 1. To compare the obtained results with the Kondo model [33, 34] and unambiguously determine Kondo temperature, we plot the square of the effective local moment $\mu_{\text{eff}}^2(T) = T\chi_s(0)$ vs. $T/T_K$, where $T_K$ is determined by the fit to the universal dependence for the Kondo model (KM) [33, 34] (black line) at low temperatures. The open black circles denote the characteristic boundaries of the “plateau” of $\mu_{\text{eff}}^2$, which is defined by the values of temperature at which $\mu_{\text{eff}}^2$ reaches 0.975 of its maximal value.

FIG. 1. Temperature dependence of the square of the effective local moment, $\mu_{\text{eff}}^2 = T\chi_s(0)$ at various values of the Coulomb interaction $U$. The Kondo temperature $T_K$ is obtained from the fit to the universal dependence for the Kondo model (KM) [33, 34] (black line) at low temperatures. The open black circles denote the characteristic boundaries of the “plateau” of $\mu_{\text{eff}}^2$, which is defined by the values of temperature at which $\mu_{\text{eff}}^2$ reaches 0.975 of its maximal value.

In Fig. 2 we show frequency dependence of local dynamic spin susceptibility $\chi_s(\omega)$ on the real frequency

$\chi_s(\omega)$ on the real frequency
axis (obtained by using Padé approximants) at various temperatures and $U = 2$. The frequency dependence of the real part of susceptibility has a form of the peak, which width reflects inverse lifetime of local moments [4]. Changing temperature from $T = 14.7T_K$ to $T = 8.5T_K$ on the plateau of $\mu_e^2$, we observe slight narrowing peak of $\chi_s(\omega)$ of the width $\sim T$. With further decrease of temperature (screening regime) the peak is strongly broadened (the local moment lifetime decreases) due to screening effects.

To study behavior of charge degrees of freedom in the local moment and screening regimes, in Fig. 3 we show temperature dependence of local charge compressibility $\chi_c(T)$. With decreasing temperature the local compressibility first increases due to increase of the coherence of quasiparticles. At lower temperatures, the decrease of local compressibility is observed, which is associated with local moment formation, cf. Refs. [20, 25]. Therefore, the position of the maximum of $\chi_c(T)$ dependence, which happens at $T_{c,\text{max}} \sim (10 \div 50)T_K$, is used in the following as a characteristic temperature of entering preformed local moment (PLM) regime. With further reducing temperature, at $T_{c,\text{min}} \sim (5 \div 10)T_K$ we observe characteristic minimum of local compressibility, which we associate with full formation of local moments, i.e. maximal portion of electrons participating in the local moment formation. Further increase of local compressibility reflects the screening of local moments (which is denoted in the following as SCR regime), occurring as a consequence of virtual transitions from local moment to itinerant states.

As we discuss in Supplemental Material [40], the increase of the local compressibility below $T_{c,\text{min}}$ is provided by the lowest (negative) eigenvalues of susceptibility $\chi^{\nu'}$ (corresponding to even in frequency eigenfunctions), which are related to the irreducible vertex divergences. We also compare [40] the above discussed temperature dependence of local compressibility to that for double occupation $\langle n_+ n_- \rangle$, which describes the average value of the square of the local spin $\langle S^2 \rangle = (3/4)(1 - 2\langle n_+ n_- \rangle)$. Similarly to local compressibility, the double occupation has a minimum at approximately the same temperatures $T_{c,\text{min}}$. Notably, the double occupation only slightly increases below $T_{c,\text{min}}$, in contrast to the local compressibility $\chi_c$, which almost recover at low temperatures its maximal value at the temperature $T_{c,\text{max}}$. This reflects the difference between electrons participating in virtual transitions and average number of electrons participated in screening. In average, only small portion of electrons can participate in screening at half filling, since most of them already form local magnetic moments. However, due to virtual transitions, substantial screening effects can be achieved at a given site of the lattice. According to the thermodynamic relation $\langle S \rangle \propto -\frac{1}{\gamma_T} \frac{\partial S}{\partial U}$ (cf. Ref. [45]), the entropy $S$ reaches local maximum as a function of $U$ at the boundary of PLM and SCR regions.

The phase diagram, summarizing the above results, is shown in Fig. 4. The obtained boundary of the beginning of the formation of local magnetic moment corresponding to the temperatures $T_{c,\text{max}}$ of maxima of local charge compressibility is qualitatively similar to the interaction dependence of the local moment formation, obtained recently in Ref. [26]. The interaction dependence of the temperatures $T_{c,\text{max}}$ repeats also qualitatively the line of $T_{c,\text{max}}$ of the Mott-Hubbard transition taken from Ref. [46] is indicated by blue line, and irreducible vertex divergences [19] are showed by yellow and orange lines.
temperature is shown in Fig. 4. For comparison, we also of the critical exponent of resistivity Mott insulator (not shown). This reminds us a change it joins with the crossover line between bad metal and U point of critical interaction U are obtained only above the interaction 

\[ T > T \] χ of minima and maxima of local compressibility diverge. Also, the first divergence line is characterized by odd in frequency eigenfunctions of the charge susceptibility \[ \chi_g \] [19], while only even in frequency eigenfunctions contribute to local compressibility (see Refs. [22–24, 47] and Supplemental Material [40]).

The temperatures \( T_{c, \min} \), corresponding to the minima of \( \chi_c(T) \), as we discuss above, determine complete formation of local magnetic moments, and separate the region of partially formed local moments (at \( T > T_{c, \min} \)) and their subsequent screening (at \( T < T_{c, \min} \)). The location of this boundary, as it is mentioned above, appears to be very close to the temperatures of the minima of the the double occupancy (green dashed line with squares); the temperatures \( T_{c, \min} \) are also sufficiently close to the low temperature boundary of the plateau of \( \mu_{\text{eff}} \). We also note that the minima and maxima of local compressibility are obtained only above the interaction \( U \), at which the first vertex divergence occurs, see also Ref. [49]. With increasing interaction the line \( T_{c, \min} \) approaches the end point of critical interaction \( U_{\text{c2}} \) of Mott transition, where it joins with the crossover line between bad metal and Mott insulator (not shown). This reminds us a change of the critical exponent of resistivity \( \rho \sim T^\beta \) from \( \beta > 2 \) to \( \beta < 2 \) at the boundary of a similar shape, located near the Widom (crossover from metal to insulator) line, discussed some time ago for frustrated magnetic systems [48]. The boundary between PLM and SCR regimes also qualitatively follows the bendings of irreducible vertex divergence lines, obtained in Ref. [19], which allows us to associate these bendings with PLM-SCR crossover.

At \( T < T_K \) Fermi liquid state of screened local moments appear; the interaction \( U \) dependence of Kondo temperature is shown in Fig. 4. For comparison, we also plot the results for the Kondo temperature from the “fingerprint” criterion, based on comparison of \( \chi_g^{\nu \nu} \) at the lowest fermionic Matsubara frequencies [25, 40]. One can see that the two definitions of Kondo temperature yield close results near the Mott-Hubbard transition, providing “universal” definition of the Kondo temperature in this regime. However, with a decrease of Coulomb interaction, the “fingerprint” criterion yields overestimate of Kondo temperature and turns into the boundary of the divergence of the irreducible vertex, obtained in Ref. [19], above the temperature of the bending of first divergence line. This shows that away from Mott transition not only lowest Matsubara frequencies contribute to screening, which reflects widening of central peak of spectral function with decreasing interaction. It is plausible to assume, that the screened state is described by some linear combination of odd in frequency eigenfunctions of the susceptibility \( \chi_g^{\nu \nu} \). This would be consistent with the fact that the local charge compressibility, which is contributed by even eigenfunctions of \( \chi_L^{\nu \nu} \), does not show any peculiarities at the Kondo temperature.

In summary, we have studied the relation between spin and charge responses in different stages of local moment formation and screening. The formation of local magnetic moment is signaled by plateau of the temperature dependence of the effective magnetic moment \( \mu_{\text{eff}} = T \chi_s(0) \), minimum of local charge susceptibility and double occupation. With further reducing temperature the local moment is screened, the effective moment decreases, while local charge compressibility and double occupation increase. Strong increase of charge susceptibility vs. weak increase of double occupation demonstrates importance of virtual transitions in local magnetic moment screening. Since local charge compressibility is affected by formation of local moment, we associate this process with contribution of even in frequency eigenfunctions of the susceptibility \( \chi_L^{\nu \nu} \). Full screening of local moment occurs at \( T < T_K \). We show that in the vicinity of Mott transition \( T_K \) is correctly described by the fingerprint criterion, while further away from the transition the latter criterion somewhat overestimates Kondo temperature.

In the present paper we neglect magnetic correlations due to the long-range order in the ground state. In this respect, the results are applicable to frustrated lattices, and can be used to describe peculiarities of the spin liquid state [50–52]. More generally, the results of the paper can be further used for description of materials with almost formed local moments, such as Hund metals, systems in the vicinity of Mott transition, etc. Analytical studies of the relation of charge and spin responses in the systems with local moments is of certain interest.

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SUPPLEMENTAL MATERIAL

to the paper “Local magnetic moment formation and kondo screening in the half filled two dimensional single band hubbard model”

1. Eigenvalues of charge susceptibility

The fermionic frequency resolved local charge susceptibility is defined by

\[
\chi_{\nu'\nu}^{\alpha\beta} = T^2 \sum_{\sigma\sigma'} \int d\tau_1 d\tau_2 d\tau_3 \left[ \langle T_\tau c_{\sigma\sigma'}^\dagger(\tau_1) c_{\sigma\sigma}(\tau_2) \right] \\
\times \chi c_{\nu'\nu}^{\alpha\beta} = \lambda_\alpha \phi_{\nu\alpha}^R \phi_{\nu'\alpha}^L.
\]

By introducing inverse (left) eigenvectors \( \phi_{\nu\alpha}^L \equiv (\phi^{-1})_{\nu\alpha} \) (taken as a matrix inverse), we find

\[
\chi_{\nu'\nu}^{\alpha\beta} = \sum_{\alpha} \lambda_\alpha \phi_{\nu\alpha}^R \phi_{\nu'\alpha}^L.
\]

Full local charge susceptibility \( \chi_c = \sum_{\nu,\nu'} \chi_{\nu'\nu}^{\alpha\beta} \) is then expressed as \( \chi_c = \sum_\alpha \chi_c^{\alpha\beta} \), where

\[
\chi_c^{\alpha\beta} = \lambda_\alpha \left( \sum_{\nu} \phi_{\nu\alpha}^R \right) \left( \sum_{\nu'} \phi_{\nu'\alpha}^L \right).
\]

According to the Eq. (A4) only eigenvalues, corresponding to the even in frequency eigenfunctions, contribute to charge susceptibility, cf. Ref. 23 of the paper. The odd in frequency eigenfunctions may however play important role in description of screening of local magnetic moment, see Sect. 3 of this Material.

One can see from Fig. S1 that the largest contributions to charge susceptibility, which originate from positive eigenvalues, are suppressed with temperature. The subleading largest contributions are however non-monotonic at the temperatures near \( T_{c,\text{max}} \), providing maximum of charge susceptibility at \( T = T_{c,\text{max}} \). The non-monotonic behavior of charge susceptibility near \( T = T_{c,\text{min}} \) is entirely related to non-monotonic behavior of lowest (negative) contributions, which originate from negative eigenvalues (corresponding to even in frequency eigenfunctions) occurring due to passing irreducible vertex divergence lines.

2. Double occupation

In Fig. S2 we show temperature dependencies of double occupations \( \langle n_+ n_- \rangle \) for various \( U \). As one can see, the double occupation decreases with decreasing temperature at \( T \gtrsim 10 T_K \). The minimum of \( \langle n_+ n_- \rangle \), which indicates the maximum of the square of the local moment, is observed at approximately the same temperatures \( T_{c,\text{min}} \), as extracted from the minima of local compressibility. Increase of double occupation with further decreasing temperature corresponds to screening of local magnetic moments.

FIG. S1. The lowest (upper plot) and largest (lower plot) contributions to charge susceptibility arranged in ascending order at various values of temperature \( T \) at the value of the Coulomb interaction \( U = 2.0 \).

FIG. S2. Temperature dependence of the double occupation for different values of the Coulomb interaction \( U \). The open black circles indicate local minima of double occupation.
3. The $2 \times 2$ fermionic frequency subspace and the “fingerprint criterion”

The “fingerprint” criterion of Ref. [25] of the paper operates with $2 \times 2$ subspace of Matsubara frequencies $\nu, \nu' = \pm \nu_1 = \pm \pi T$ and reads $\chi^{\nu_1,\nu_1}_c = \chi^{\nu_1,-\nu_1}_c$. As we argue in the main text, this criterion is applicable near Mott transition, where in the vicinity of the Kondo temperature $T \lesssim T_K$ one can restrict consideration by the above mentioned subspace, which corresponds physically to the quite narrow width of central (quasiparticle) peak of the spectral function. On the other hand, at sufficiently high temperatures $T \gtrsim T_{c,\text{max}}$ one can also restrict consideration to the abovementioned subspace since larger Matsubara frequencies give irrelevant contribution in that regime, cf. Ref. [19] of the paper.

In the above mentioned subspace we have

$$
\phi_{\nu,1}^R = \phi_{\nu,1}^L = (1, 1)/\sqrt{2}, \\
\phi_{\nu,2}^R = \phi_{\nu,2}^L = (1, -1)/\sqrt{2}
$$

(A5)

with eigenvalues $\lambda_{1,2} = \chi_c^{\nu_1,\nu_2} \pm \chi_c^{\nu_1,-\nu_1}$. The charge susceptibility within the considered subspace $\chi_c = 2\lambda_1$ is determined only by the eigenvalue $\lambda_1$. The eigenvectors $\phi^{R,L}_{\nu,1}$, which affect fermionic frequency summed charge susceptibility $\chi_c$ can be therefore related to the formation of local moment. At the same time, the eigenvalue $\lambda_2$ vanishes when the “fingerprint” criterion of Kondo screening is fulfilled. The corresponding eigenvectors $\phi^{R,L}_{\nu,2}$ can be therefore considered as responsible for the local moment screening near Mott transition. The antisymmetry of these vectors with respect to frequency may reflect the so called orthogonality theorem [1]. Interestingly, the same antisymmetric vectors $\phi^{R,L}_{\nu,2}$ were recently used in Ref. [47] of the paper for constructing Landau functional of Mott transition, which is also related to disappearance of quasiparticle peak.

In discussing the phase diagram of Fig. 4 of the paper we conjecture that the conclusions from the considered $2 \times 2$ frequency subspace on the parity of relevant eigenfunctions in various regimes remain valid in broader range of $U$ in the strong coupling regime, where broader fermionic frequency range becomes important.

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