Coherence scale of the two-dimensional Kondo Lattice model.

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A doped hole in the two-dimensional half-filled Kondo lattice model with exchange $J$ and hopping $t$ has momentum $(\pi, \pi)$ irrespective of the coupling $J/t$. The quasiparticle residue of the doped hole, $Z_{m, c}$, tracks the Kondo scale, $T_K$, of the corresponding single impurity model. Those results stem from high precision quantum Monte Carlo simulations on lattices up to $12 \times 12$. Accounting for small dopings away from half-filling within a rigid band approximation, this result implies that the effective mass of the charge carriers at the Fermi level tracks $1/T_K$ or equivalently that the coherence temperature $T_{coh} \propto T_K$. This results is consistent with the large-N saddle point of the $SU(N)$ symmetric Kondo lattice model.

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In a Fermi liquid, the coherence scale corresponds to the energy scale below which thermodynamic properties are determined by the Fermi surface: the specific heat is linear in temperature and the spin charge uniform susceptibilities temperature independent. This scale is inversely proportional to the effective mass of the charge carriers. In this article, our aim is to compute the coherence scale in models of heavy fermion materials [1]. Our starting point is the Kondo Lattice model (KLM),

$$H = -t \sum_{\langle i,j \rangle, \sigma} [c_{i, \sigma}^\dagger c_{j, \sigma} + \text{h.c.}] + J \sum_i \tilde{S}_i^c \tilde{S}_i^f, \tag{1}$$

on a square lattice. The first term describes a band of non-interacting electrons in a tight binding approximation ($c_{i, \sigma}^\dagger$ creates an electron in a Wannier state centered around lattice site $i$ with $z$-component of spin $\sigma$) and the sum runs over nearest neighbors. The spin degrees of freedom of the conduction electrons, $\tilde{S}_i^c = \frac{1}{2} \sum_{s,s'} c_{i,s}^\dagger \sigma_{s,s'} c_{i,s'}^\dagger$ with $\sigma$ the Pauli spin matrices, interact antiferromagnetically, $J > 0$, with a lattice of spin $1/2$ magnetic impurities, $\tilde{S}_i^f$. The KLM at $J/t \ll 1$ stems from the periodic Anderson model (PAM) in the limit where charge fluctuations are negligible.

In the limit of a single impurity, the model is well understood: at high temperatures the impurity spin is essentially free and at low temperatures it is screened via the formation of a many body singlet state of the conduction electrons and impurity spin. The characteristic, universal, energy scale describing this crossover from the free to the screened magnetic impurity is the Kondo temperature, $T_K$ [2]. In the lattice case, it is appealing to view the heavy fermion metallic state as a consequence of a coherent, Bloch-like, superposition of individual Kondo screening clouds. The coherence scale of the metallic state has been investigated in details within the large-N approximation for the KLM [3] and the dynamical mean field approximation for the related PAM [4]. Both approaches yield $T_{coh} \propto T_K$ as a function of $J/t$ with a proportionality factor depending strongly on the band-filling. Since both approximations neglect spatial fluctuations, they do not capture the Ruderman-Kittel-Kasuya-Yosida (RKKY) interaction which introduces a new energy scale into the problem and drives the ground state through a magnetic order-disorder quantum phase transition. The new result in this Letter is that the relation $T_{coh} \propto T_K$ still holds when the two-dimensional KLM is solved numerically exactly by means of quantum Monte Carlo (QMC) simulations.

To tackle this problem, we have to adopt an indirect route since the sign problem inhibits simulations away from half-filling. We hence investigate the problem of a single-hole doped into the Kondo insulating state at half-filling and then assume a rigid band to deduce the properties of the metallic state at weak dopings. In the following, we describe our approach for the $SU(2)$ symmetric model where in the limit $N \rightarrow \infty$ a paramagnetic saddle point approximation becomes exact. We then compare the obtained results with QMC simulations for the $SU(2)$ model of Eq. (1).

Mean Field. The mean field we consider neglects magnetic fluctuations triggered by the RKKY interaction but describes the Kondo effect as well as the formation of the heavy electron state. The decoupling is based on the equation: $\tilde{S}_i^c \tilde{S}_i^f = \frac{1}{4} \left( D_i^f D_i^c + D_i^c D_i^f \right)$ with $D_i = \sum_{\sigma} c_{i, \sigma}^\dagger f_{i, \sigma}$. Here, $\tilde{S}_i^c = \frac{1}{2} \sum_{s,s'} f_{i,s}^\dagger \sigma_{s,s'} f_{i,s'}^\dagger$, and $f_{i, \sigma}$ are fermionic operators. At the mean-field level one adopts a real order parameter, $r = (D_i^f)$, and the constraint of a single charge per f-site is imposed on average via a Lagrange multiplier $\lambda$. This mean field theory has been discussed extensively in [3]. Here, we will concentrate on the $J$ dependence of scales for a half-filled particle-hole symmetric conduction band. This symmetry pins the chemical potential to $\mu = 0$ and $\lambda = 0$. Single particle properties are derived from the Green function $G(\tilde{r}, i\omega_n) = 1/[i\omega_n - \epsilon(\tilde{r}) - \Sigma(i\omega_n)]$ with self-energy

$$\Sigma(i\omega_n) = \frac{(Jr/2)^2}{i\omega_n} \tag{2}$$

and $\epsilon(\tilde{r}) = -2t (\cos(k_x) + \cos(k_y))$. Assuming a flat density of states, $D(\epsilon)$, of width $W$ satisfying $\int d\epsilon D(\epsilon) = 1$ and $D(\epsilon) = D(-\epsilon)$ we can solve the saddle point equa-
tions to obtain:

\[ r(T = 0) = \frac{W}{2J \sinh(W/2J)}. \]  

(3)

The order parameter \( r \) vanishes at the Kondo temperature \( T_K \). At the mean-field level, this energy scale is independent on the impurity concentration and hence matches the Kondo temperature of the corresponding single impurity problem. With the above flat density of states we obtain:

\[ T_K \propto W e^{-W/J} \propto 1 \left( J r(T = 0) \right)^2 \text{ for } J/t << 1. \]  

(4)

The functional form of the self-energy leads to the dispersion relation \( E_{\vec{k}} = \frac{1}{2} \left[ \epsilon(\vec{k}) - \sqrt{\epsilon^2(\vec{k}) + (J r)^2} \right] \) with residue \( Z_\vec{k} = \frac{1}{2} \left[ 1 - \epsilon(\vec{k}) \right] / \sqrt{\epsilon^2(\vec{k}) + (J r)^2} \) for a doped hole away from half-filling. At \( T = 0 \) and in the weak-coupling limit, both the quasiparticle gap, \( \Delta_{qp} = \mu - E_{\pi,\pi} \), and residue track the same scale:

\[ \Delta_{qp} \propto Z_{(\pi,\pi)} \propto \left( J r(T = 0) \right)^2 \propto T_K \text{ for } J/t << 1. \]  

(5)

Under a rigid band assumption (see Discussion section) this results implies that the coherence temperature of the metallic state at small hole dopings away from half-filling tracks the Kondo scale. At the mean-field level this statement may be checked explicitly by solving the mean-field approach formally. Hence it is a-priori not clear that the scales described by the mean-field approximation survive when the model is solved exactly.

\[ -G(\vec{k}, -\tau) = \langle \Psi_0^N | \epsilon_{\vec{k},\sigma}^\uparrow (\tau) \Psi_{\vec{k},\sigma}^N \rangle \tau \rightarrow \infty \propto Z_\vec{k} e^{-\Delta_{qp}(\vec{k}) r} \]  

(6)

since \( Z_\vec{k} = \left| \langle \Psi_0^N | \epsilon_{\vec{k},\sigma}^\uparrow | \Psi_{\vec{k},\sigma}^{N-1} \rangle \right|^2 \). Clearly high precision results are required to extract the residue. Fig. 1 plots typical raw data. To reach such precision we use a newly developed method for the calculation of \( G(\vec{k}, \tau) \) within the PQMC [4].

**Numerical Results.** In numerical simulations of the two-dimensional KLM, the RKKY interaction triggers a magnetic order-disorder quantum phase transition at \( J_c/t = 1.45 \pm 0.05 \) [5]. The question then arises if the antiferromagnetic ordering destroys Kondo screening and hence the possible appearance of a Kondo scale in the numerical data. We answer this question by analyzing the single particle spectral function. Assuming that well under \( J_c/t \) the impurity spins are frozen into their antiferromagnetic ordering, we can use the mean-field Ansatz, \( S_i^{\uparrow,\downarrow} = \frac{1}{2} m_i \epsilon_i^{\uparrow,\downarrow} \), which leads to a single hole dispersion relation: \( E(\vec{k}) = -\sqrt{\epsilon^2(\vec{k}) + (J/4)^2} \) [8]. This approximation correctly reproduces the quasiparticle gap \( \Delta_{qp} \propto J/4 \) in the small \( J \) limit (see Fig. 3) but fails to account for the observed dispersion relation in the spectral function. This statement is based on comparison with QMC data: the thin vertical lines in Fig. 2 tracking the dispersion relation \( -\sqrt{\epsilon^2(\vec{k}) + (J/4)^2} \) do not account for the low energy features around the \((\pi, \pi)\) point. On the other hand, comparison with the mean-field approximation of the previous section (bold vertical lines in Fig. 2), allows the interpretation that the low-lying features in the vicinity of \( \vec{k} = (\pi, \pi) \) stem from Kondo screening and are shifted to energy scales of order \( J/t \) due to the onset of magnetic ordering. We have checked that this functional form of the dispersion relation survives down to \( J/t = 0.2 \) on \( 8 \times 8 \) lattices. In the magnetically ordered phase, a doped hole at \( \vec{k} = (\pi, \pi) \) can scatter off a gapless magnon with momentum \( \vec{Q} = (\pi, \pi) \) thus generating a shadow feature at \( \vec{k} = (0, 0) \). Upon close inspection, such features are seen in Fig. 2. The quasiparticle dispersion relation is at best described in terms of partial Kondo screening of the impurity spins. The remnant non-screened moment orders antiferromagnetically [8, 10].

Our major concern is the quasiparticle residue at \( \vec{k} = (\pi, \pi) \). In Fig. 3 we plot this quantity as a function of

![FIG. 1: Zero temperature Green function defined in Eq. 6. Fitting the tail of this quantity to the form \( Z_\vec{k} e^{-\Delta_{qp}(\vec{k}) r} \) yields the quasiparticle residue and quasiparticle gap at wave vector \( \vec{k} \).](image-url)
A($\vec{k}$; $\omega$), $J/t = 0.8$

\begin{align*}
A(\vec{k}; \omega), J/t = 0.8
\end{align*}

$A(\vec{k}; \omega)$, $J/t = 0.8$

$J/t$ for 8 × 8 and 12 × 12 lattices. At small values of $J/t$ size effects become more and more important. For $J/t = 0.4$ and 0.8 we have extrapolated the data to infinite sizes by fitting the $L = 4, 6, 8, 12$ QMC results to the form $a + b/L + c/L^2$. To compare this scale to the single impurity Kondo scale, we have carried out simulations of

\begin{align*}
H = \sum_{\vec{k},\sigma} \epsilon(\vec{k}) c_{\vec{k},\sigma}^\dagger c_{\vec{k},\sigma} + J \vec{S}_I \vec{S}_f
\end{align*}  

(7)

with a standard implementation of the Hirsch-Fye QMC algorithm [11]. In this algorithm the CPU time scales as $\beta^3 N^0$ where $N$ corresponds to the number of lattice sites and $\beta$ to the inverse temperature. This scaling behavior allows one to carry out simulations on arbitrarily large lattices but limits the accessible temperature range. Form the data collapse of the impurity spin susceptibility (see Fig. 4) we can extract the Kondo temperature for our given band structure. Note that the so obtained Kondo temperature (triangles in Fig 3) compares remarkably well with the mean-field value (solid line in Fig. 3).

At small values of $J/t$ ($J/t = 0.4$) the Kondo temperature is too small to compute with the Hirsch-Fye algorithm and we have to rely on the mean-field result to compare with the lattice QMC results.

The data of Fig. 3 show several features.

i) The major observation is that within the considered range of coupling constants the QMC results are consistent with

\begin{align*}
Z_{(\pi,\pi)} \propto T_K.
\end{align*}  

(8)

ii) Due to the occurrence of antiferromagnetic order below $J_c/t = 1.45 \pm 0.05$, the quasiparticle gap tracks $J$. 

FIG. 2: Single particle spectral function as obtained from analytically continuing the imaginary time QMC data with the Maximum Entropy method. The single particle occupation numbers, $n_{\vec{k}} = \sum_\sigma \langle c_{\vec{k},\sigma}^\dagger c_{\vec{k},\sigma} \rangle$, are listed on the left hand side of the plot, and correspond to the weight under each spectrum: $\pi n_{\vec{k}} = \int_0^\infty d\omega A(\vec{k}, \omega)$. The thin vertical lines track the dispersion relation of hole in a static staggered magnetic field (see text): $-\sqrt{\epsilon^2(\vec{k}) + (J/4)^2}$. The bold vertical lines correspond to the dispersion relation stemming from the self-energy of Eq. 2 with the order parameter $r$ determined self-consistently.

FIG. 3: Scales as a function of $J/t$ as determined from QMC simulations (see text). The data for the quasiparticle gap are a result of extrapolation to the thermodynamic limit. The solid line corresponds to the mean-field (see section Mean-field) value of the Kondo temperature. Within our resolution we cannot distinguish it from the QMC value.
magnetic order-disorder phase transition (iii) Within our resolution and limitation in lattice size, we survive.

\[ \chi = \int_0^\beta d\tau \langle ml(\tau)ml(0) \rangle, \]
for the Kondo model as determined with a standard implementation of the Hirsch-Fye algorithm. From the collapse of the data, we can estimate the Kondo temperature for the listed values of \( J/t \).

Even in the presence of this large quasiparticle gap, the Kondo-like features in the single-hole spectral function—flat band around the \((\pi, \pi)\) point with \( Z_{(\pi, \pi)} \propto T_K \)—survive.

iii) Within our resolution and limitation in lattice size, we observe no anomaly in the quasiparticle residue across the magnetic order-disorder phase transition \((J_c/t \simeq 1.45)\).

**Discussion** Under the assumption of a rigid band, the result of Eq. 8 has important implications. Since the quasiparticle gap is determined by the \((\pm\pi, \pm\pi)\) points in the Brillouin zone, infinitesimal hole doping away from half-filling yields a metallic state with Fermi surface consisting of hole pockets centered around the \((\pm\pi, \pm\pi)\) \( k \)-points. This leads to a Fermi surface with large Luttinger volume containing both conduction and impurity electrons. The effective mass of this Fermi liquid at infinitesimal hole dopings is inversely proportional to the quasiparticle residue:

\[ m^* \propto \frac{1}{Z_{(\pi, \pi)}}, \quad \text{(9)} \]

The coherence temperature, \( T_{\text{coh}} \), is inversely proportional to the effective mass. Hence Eq. 9 along with our QMC result of Eq. 6 is equivalent to

\[ T_{\text{coh}} \propto T_K. \quad \text{(10)} \]

Let us comment on the implicit assumptions lying behind the above equation.

i) Support for the rigid band assumption follows from the fact the Kondo insulator is adiabatically linked to band insulator realized in the non-interacting periodic Anderson model. This stands in contrast to the Mott insulating state.

ii) That the effective mass is inversely proportional to quasiparticle residue implicitly assumes that the enhancement of \( m^* \) is driven by the frequency dependence of the self-energy. We can obtain support for this statement by computing the effective mass as the inverse curvature of the dispersion relation around \( \vec{k} = (\pi, \pi) \) thus capturing the mass enhancement origination from the frequency as well as momentum dependence of the self-energy. Within our accuracy, this quantity tracks \( 1/Z_{(\pi, \pi)} \) as a function of \( J/t \) thus confirming the validity of our assumption.

In conclusion, we have carried out high precision QMC calculations of the half-filled KLM on a square lattice. We have shown that from weak to strong coupling and across the magnetic quantum phase transition, a doped hole has momentum \((\pi, \pi)\) and quasiparticle residue which tracks the Kondo scale of the corresponding single impurity model. Assuming a rigid band, this result leads to the conclusion that the \( J \)-dependence of coherence scale in the metallic state at small dopings away from half-filling tracks the Kondo scale. Since this result compares favorably with large-N and dynamical mean-field theories which omit spatial fluctuations, we can follow the idea that the coherence scale is insensitive to the RKKY magnetic scale.

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