Anomalous properties of the Hubbard model in infinite dimensions

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Anomalies are found in the resistivity ρ and NMR rate $1/T_1$ of the infinite-dimensional Hubbard model using quantum Monte Carlo calculations and the noncrossing approximation. For temperatures greater than the "Kondo scale" T_0, we obtain $1/T_1 \sim a+bT$ and $\rho \sim c+dT$ (a, b, c, d constants). For temperatures $T \ll T_0$ we infer from a saturation of the effective mass of the carriers that the ground state of the system is a Fermi liquid.

Since the discovery of the high-T_c oxide superconductors,[1] one of the most fascinating problems is a microscopic explanation of their unconventional normal-state properties:[2] A linear resistivity $\rho \sim T$ and NMR relaxation $1/T_1 \sim a+bT$ are the most prominent anomalous features common to these compounds. In this paper we demonstrate (see Figs. 3 and 4) that the infinite-dimensional Hubbard model also displays these anomalies while retaining a Fermi-liquid ground state.

A comparison of the different relevant electronic energy scales in the cuprates suggests that the motion of the electrons is confined to the CuO planes and subject to strong local Coulomb interactions; i.e., these materials belong to the class of so-called strongly correlated electron systems.[3] Since such anomalous normal-state properties cannot be obtained from the usual Fermi-liquid picture, it was from the very beginning conjectured by theorists that they are rather directly related to an interplay of this two-dimensional (2D) character and the strong correlations.[3,4] In particular, the possibility of the occurrence of a non-Fermi-liquid ground state is intensively discussed.

In order to describe the relevant planar electronic degrees of freedom microscopically, they may be mapped on a model well known to solid-state theorists, namely, the single-band Hubbard model.[5,6] Using standard notation, the Hubbard Hamiltonian in D dimensions reads[5]

$$\mathcal{H} = -\frac{t^*}{2\sqrt{D}} \sum_{\langle ij \rangle,\sigma} (C^\dagger_{i,\sigma} C_{j,\sigma} + C^\dagger_{j,\sigma} C_{i,\sigma}) + \sum_i [\epsilon(n_{i,\uparrow}+n_{i,\downarrow}) + U(n_{i,\uparrow}-\tfrac{1}{2})(n_{i,\downarrow}-\tfrac{1}{2})] \;, \quad (1)$$

where $C_{i,\sigma}$ ($C^\dagger_{i,\sigma}$) destroys (creates) an electron of spin σ on site i of a hypercubic lattice of dimension D, $n_{i,\sigma} = C^\dagger_{i,\sigma} C_{i,\sigma}$, and we choose our unit of energy so that $t^* = 1$.

In view of the anomalous properties of the cuprates, the expectations for the 2D Hubbard model are especially controversial: Is it a "normal" Fermi liquid renormalized by a coupling to strong spin fluctuations,[7] a Luttinger liquid[8] known from the extreme limit of 1D, or rather something in between, a so-called "marginal" Fermi liquid?[4] The discussion of these problems is further complicated by the fact that despite the simplicity of the model, no exact solutions exist except in one dimension, where the knowledge is in fact rather complete.[9] The extent that this very special limit can serve as a reference point for any model with $D > 1$ (Refs. 8 and 10) remains however, controversial, and an examination of the model from a different point of view is clearly needed.

Recently, an approach[11-13] based on an expansion in $1/D$ about the point $D = \infty$ has been proposed to study such strongly correlated lattice models. In this limit the requirement of a finite total energy per site makes it necessary to rescale nonlocal interactions by an appropriate power of D^{-1}.[11,12] While, e.g., spin exchange will essentially reduce to the corresponding mean-field-theory results,[12] interactions such as the screened Coulomb repulsion in the model (1) remain nontrivial even in this limit. This especially means that the essential local dynamics remain unaltered.

The basic idea of our approach is to map the infinite-dimensional Hubbard model onto a self-consistently embedded Anderson impurity.[14,15] Then either the quantum Monte Carlo (QMC) algorithm of Hirsch and Fye[16] or the finite-U noncrossing approximation[17] (NCA) is used to solve the impurity problem. Details of this algorithm have been described previously. Results from the NCA are compared to the (essentially exact) QMC results to determine where the NCA is valid to within a few percent or less.[18] The NCA is used since it easily produces single-particle dynamic results, whereas one must analytically continue the QMC data to obtain dynamics. Especially for nonlocal quantities such as transport, this analytic continuation is computationally expensive. However, it is relatively easy to produce local dynamic quantities such as NMR or single-particle density of states (DOS) by analytically continuing the QMC results. Thus all static quantities (i.e., susceptibilities) as well as local dynamic quantities (DOS, NMR) were produced with the QMC method. Nonlocal dynamics such as transport

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were calculated with the NCA, with a limited set of calculations performed with the QMC algorithm to determine the region of validity of the NCA results.

In previous publications,[19,20] we presented an exact numerical solution of the Hubbard model in the infinite-dimensional limit. We will first summarize those results: At half filling $\delta = 1 - \langle n \rangle = 0$, for $U \gtrsim 3.5$, the single-particle DOS develops a pseudogap[19] and the effective mass diverges. The ground state of the half-filled model is always an antiferromagnet. When the model is hole doped ($\epsilon > 0$) away from half filling, the commensurate antiferromagnetism is quickly suppressed, yielding to an incommensurate state when $\delta \gtrsim 0.15$. As doping continues beyond this point, transitions, if any, become difficult to detect with the QMC method because of extremely low transition temperatures. In the paramagnetic region, the system becomes a heavy metal characterized by a narrow peak of width $\approx T_0$ in the single-particle density of state near the Fermi surface.[20] The development of this peak is associated with a screening of the local moments and the enhancement of the effective electron mass.[20] Hence we associate the peak with the Kondo effect and its width T_0 with the Kondo scale.

In this paper we study the properties of the infinite-dimensional Hubbard model away from half filling as a function of doping. In particular, we show that for dopings typical of the oxide superconductors, the model exhibits an anomalous NMR (Fig. 3) and transport (Fig. 4) as described before. At the same time, the ground state of the model appears to be a (moderately heavy) Fermi liquid (Fig. 2). Throughout the paper we concentrate on a value for the Coulomb repulsion, $U = 4$. This value appears to be most appropriate when comparing our results to experiment; however, the *qualitative* features of our results do not depend on U as long as $U \gtrsim 3.5$.

Scaling. For low temperatures ($T \lesssim T_0$), we find that many of the physical properties of the system—magnetic susceptibilities (see inset to Fig. 1), NMR, transport, specific heat—appear to show some scaling with T/T_0. Since the $D = \infty$ model may be mapped onto an (effective) Anderson impurity, we can use a similar method to define this scale T_0: T_0 is fixed by the zero-temperature local susceptibility $\chi_{ii}(T=0) = 1/T_0$. This is shown in Fig. 1 where $1/T_0\chi_{ii}(T)$ is plotted versus T/T_0. The relative values of T_0 were chosen to cause the data sets for different doping to coincide, whereas the magnitude was fixed by demanding that the y intercept (determined by a quadratic extrapolation) be 1. T_0 increases in a weakly superlinear fashion with δ. T_0 along with several other relevant parameters (to be discussed later) are presented in Table I.

Fermi-liquid properties. To examine whether the zero-temperature fixed point of the $D = \infty$ Hubbard model is a Fermi liquid or not, one may calculate the finite-temperature quasiparticle renormalization factor as defined by Serene and Hess,[21] $a^{-1}(T) = 1 - \mathrm{Im}\sum(i\omega_0)/\omega_0$. In Fig. 2 the renormalization factor is plotted versus T/T_0 when $U = 4$ and $\delta = 0.1878$. Three different regions may be identified in this data: In the *Fermi-liquid regime* $T \ll T_0$, $a^{-1}(T)$ appears to saturates to a finite value as the temperature is reduced below T_0, indicating

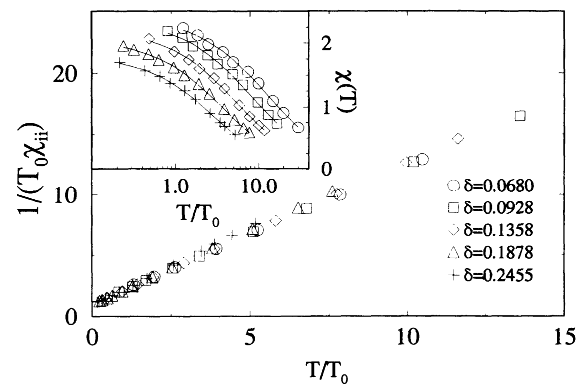

FIG. 1. Scaled local susceptibility of the Anderson impurity vs T/T_0 for several different dopings when $U = 4$. The relative values of T_0 for the different dopings were determined by causing the different curves to coincide, whereas the absolute magnitude was fixed by setting $1/(T_0\chi_{ii}(0)) = 1$. In the inset, the bulk susceptibility appears to scale with T/T_0, up to an additive constant.

the formation of a Fermi liquid.[22] The zero-temperature limit of $a^{-1}(T)$ may be estimated by extrapolation, and it gives the effective mass for the quasiparticles of this Fermi liquid, $m^*/m = a^{-1}(0)$. The mass enhancement plotted as a function of δ is shown in the inset to Fig. 2. For fixed U, the effective mass appears to diverge continuously as half filling is approached. In the *high-temperature regime* $T \gg T_0$, the Kondo peak disappears[20] and $a^{-1}(T) \to 1$ as in the free metal. The physical properties no longer show scaling. In the *crossover regime* $T \approx T_0$, $a^{-1}(T)$ increases in a roughly logarithmic linear fashion. This behavior $a^{-1}(T) \sim \ln(T)$ has been identified[21] as a signal of marginal Fermi-liquid behavior.[4] Let us stress, though, that this special behavior appears only as a crossover feature from a high- to a low-temperature regime and does not appear to persist as an anomalous ground state.

NMR. The local NMR rate

$$1/T_1 = T \lim_{\omega \to 0} \chi''(\omega)/\omega \tag{2}$$

is calculated by direct analytic continuation of the local dynamic susceptibility $\chi''(\omega)$. At temperatures $T \gtrsim 2T_0$, the NMR displays anomalous behavior such that $1/T_1 \sim aT/T_0 + b$. In Fig. 3, the solid lines are the result of a linear fit of $1/T_1 = at/T_0 + b$ to the anomalous data (the resulting values of a and b are tabulated in Table I). The anomalous region extends roughly from $T_0 \lesssim T \lesssim 10T_0$ and thus is much more pronounced for

TABLE I. Values of T_0, a, and b for different dopings when $U = 4$.

$\delta = 1 - \langle n \rangle$	T_0	a	b
0.0680	0.0177	−0.41	15.0
0.0928	0.0273	−0.20	10.1
0.1358	0.0478	−0.02	6.1
0.1878	0.0730	0.16	3.8
0.2455	0.1074	0.22	2.5

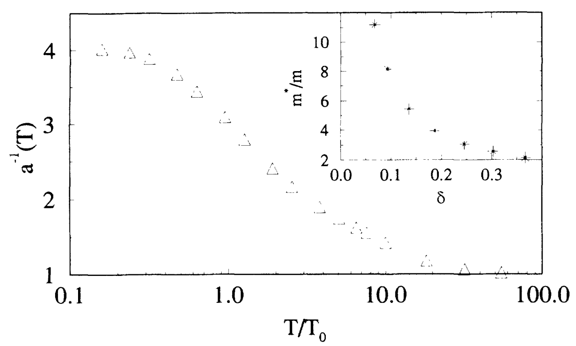

FIG. 2. Quasiparticle renormalization $a^{-1}(T)$ vs T/T_0 when $\delta=0.1878\pm0.001$ and $U=4$. In the inset the mass enhancement $m^*/m=a^{-1}(0)$, roughly estimated by extrapolation, is plotted vs δ when $U=4$.

larger doping with correspondingly larger values of T_0. The behavior in the anomalous region is only partially universal. Both a and b change with doping, with a being negative when the doping approaches zero, becoming positive and less sensitive to doping as the system is doped away from half filling. Thus, for low doping, when a is negative $1/T_1$ displays a maximum at roughly $T=T_0$. The parameter a does not show any obvious scaling with T_0. The parameter and b, on the other hand, is positive definite and to a very good approximation $b\propto 1/T_0$.

Such anomalies of $1/T_1$ have been observed for Cu NMR in the normal state of the cuprate superconductors. For example, in $YBa_2Cu_3O_7$ the Cu $1/T_1$ may be fit to a linear form from about 125 to 410 K.[23] For lower T, it falls sublinearly, and finally the data are cut off by the superconducting transition. By fitting our results to the experimental data, we estimate that $T_0\approx 150$ K in $YBa_2Cu_3O_7$. Similar behavior is seen in the 60 K $YBa_2Cu_3O_{7-y}$; however, b is considerably larger here, consistent with what would be expected as the doping is reduced. Recently, Imai *et al.*[24] studied the behavior of $1/T_1$ as a function of x in $La_{2-x}Sr_xCuO_4$. They find that their curves of $1/T_1$ versus T show negative slope for low dopings $x=0,0.04,0.075$, with one curve ($x=0.075$) showing a modest maximum (the two other data sets were not reported down to low temperatures). At larger x, the slope of $1/T_1$ versus T is positive.

Resistivity. As discussed in the beginning, the resistivity was calculated with the NCA, with the QMC results (solid symbols in Fig. 4) used only as a check to determine the range of validity of the NCA. The resistivity may be constructed from the simplest bubble diagram composed of two single-particle propagators since there are no vertex corrections in the infinite-dimensional limit.[25] A systematic test of the NCA's ability to produce single-particle and thermodynamic results was presented elsewhere.[18] There we found that the NCA was quite accurate for temperatures $T>2T_0$. Here we restrict our result to these temperatures.

In Fig. 4 the resistivity is plotted versus T for several different dopings when $U=4$. Note that the region where the resistivity is linear in T increases with doping, i.e., with T_0, Recently, Takagi *et al.*[26] performed a systematic study of the resistivity as a function of x in $La_{2-x}Sr_xCuO_4$. They found strikingly similar behavior in the planar resistivity: The region of linearity increases with doping while the slope decreases. As shown in the inset to Fig. 4, the slope of the linear region varies with δ^{-1}, an observation which is also consistent with $La_{2-x}Sr_xCuO_4$ experimental data.[27] We also find (not shown) that the resistivity scales with $(T/T_0)^2$ at low temperatures, as expected of a Fermi liquid.

Conclusion. We have explored the NMR and resistivity of the infinite-dimensional Hubbard model away from particle-hole symmetry. We find that both the NMR rate $1/T_1$ and the resistivity $\rho(T)$ have regions of linearity when plotted versus temperature. These regions of linearity increase in duration as the doping increases and are very pronounced for values of $\delta=1-\langle n\rangle\gtrsim 0.15$, consistent with the experimental observations. We would like to emphasize that our approach is *nonperturbative*; i.e., the anomalies found are indeed intrinsic to the model are *not* related to possibly lacking contributions to a perturbation theory. It thus seems clear that at least in order to explain the anomalous normal-state properties of the high-T_c superconductors *above* T_c it is not necessary to resort to exotic ground states of correlated models in 2D. Results for quantities such as the Hall effect and op-

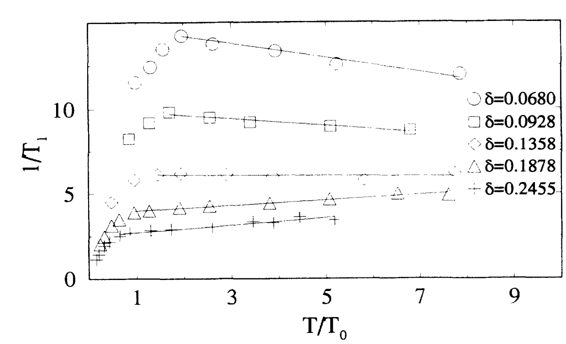

FIG. 3. $1/T_1$ vs T/T_0 when $U=4$. The solid lines are linear fits $1/T_1=aT/T_0+b$ to the data in the crossover region. Values of a and b obtained from the fit are tabulated in Table I.

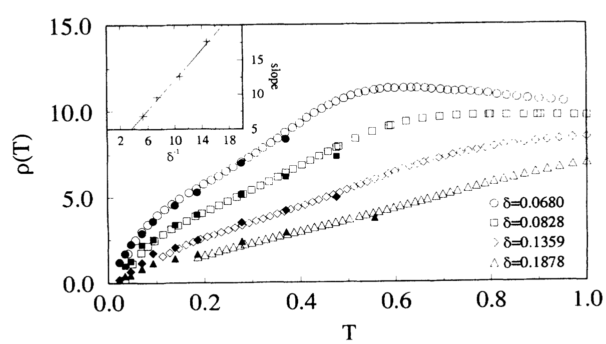

FIG. 4. Resistivity vs temperature T for various δ. The open (solid) points are calculated with the NCA (QMC algorithm). The inset shows the variation of the slope of the linear region with doping δ.

tical conductivity not presented here further support this picture. Work on these quantities is in progress and is planned to be presented in a forthcoming publication.

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