Transport Properties of the Infinite Dimensional Hubbard Model

Th. Pruschke, D.L. Cox

*Department of Physics, The Ohio State University, Columbus, Ohio 43210-1106*

M. Jarrell

*Department of Physics, University of Cincinnati, Cincinnati, Ohio 45221-0011*

(Received )

Results for the optical conductivity and resistivity of the Hubbard model in infinite spatial dimensions are presented. At half filling we observe a gradual crossover from a normal Fermi-liquid with a Drude peak at $\omega = 0$ in the optical conductivity to an insulator as a function of $U$ for temperatures above the antiferromagnetic phase transition.

When doped, the “insulator” becomes a Fermi-liquid with a corresponding temperature dependence of the optical conductivity and resistivity. We find a $T^2$-coefficient in the low temperature resistivity which suggests that the carriers in the system acquire a considerable mass-enhancement due to the strong local correlations. At high temperatures, a crossover into a semi-metallic regime takes place.

PACS numbers: 71.30.h, 72.15.-v, 72.20.-i

Typeset Using REVTEX
The one-band Hubbard Hamiltonian on a simple (hyper-)cubic lattice \[1\]

\[ H = -\sum_{(ij),\sigma} t_{ij} \left( c_{i,\sigma}^{\dagger} c_{j,\sigma} + \text{h.c.} \right) - \mu \sum_{i\sigma} n_{i\sigma} + U \sum_{i} n_{i,\uparrow} n_{i,\downarrow}, \]

where \( t_{ij} \) is restricted to nearest neighbours, is from its structure one of the simplest models in condensed matter physics. It is generally believed to contain the essential physics necessary to qualitatively describe the properties of transition metal oxides and possibly the normal state of the high temperature superconductors. Although a lot of work has been invested over the years \[2\], a reliable or even exact description of the physical properties of the Hubbard model (1) for general values of its parameters could not be achieved except for the limit of one spatial dimension \[3\]. Especially the interesting issues of a possible metal-insulator transition or unconventional low temperature phases \[1,3\] still remain unanswered.

A breakthrough towards a better understanding of highly correlated systems in general, and the Hubbard model (1) in particular, was achieved by the introduction of the limit of infinite spatial dimensions \( d \to \infty \) \[6\]. In this limit the dynamics of the system become essentially local \[7\], which considerably simplifies the task of calculating quantities of interest \[8-13\]. A particularly interesting result is that the one particle self energy \( \Sigma(k, z) \) becomes purely local \[6\]. Consequently one can map the thermodynamic potential, and thus the solution of the model (1), onto an effective Anderson impurity problem \[8-11\]. Recently, this method has been used by the present authors for a detailed study of the phase diagram \[10,12\] and thermodynamic and transport properties \[13\] of the Hubbard model using different approaches to solve the underlying impurity problem \[13\].

In this letter we give a brief description of our results for the optical conductivity and resistivity of the Hubbard Hamiltonian in the limit \( d \to \infty \). In particular, we want to address the abovementioned issues of a possible metal-insulator transition and what kind of low temperature behaviour the Hubbard model shows close to half filling and at realistic values of \( U \) in an artificially stabilized paramagnetic phase. It must be stressed that the latter constraint is essential since the Hubbard model always undergoes an antiferromagnetic transition close to half filling for sufficiently low temperatures \[10,12\]. Before turning to a
detailed discussion of our results let us give a brief summary: At half filling, one indeed encounters a crossover from a normal metal with a Drude peak in the optical conductivity at small values of the Coulomb parameter $U$ to an “insulator” with essentially zero dc-conductivity at large $U$. In addition, a charge excitation peak at $\omega = U$ develops with increasing $U$ arising from the field-induced transitions from the lower Hubbard band (LHB) to the upper Hubbard band (UHB). Off half filling, we always find a Fermi-liquid at low temperatures. However, the corresponding Fermi-liquid parameter are strongly enhanced and the resistivity shows nonmonotonic behaviour with a maximum at higher temperatures. The optical conductivity, on the other hand, has a strongly temperature dependent Drude peak and again the additional charge excitation peak at $\omega \approx U$.

In linear response theory the conductivity can be expressed as

$$
\sigma(\omega) = \text{Re} \left\{ \frac{1}{i \omega} \sum_{\mathbf{k}, \mathbf{k}', \sigma} \sum_l v_{k_l} v_{k'_l} \langle \langle n_{\mathbf{k}\sigma} n_{\mathbf{k}'\sigma} \rangle \rangle z \right\}_{z = \omega + i \delta},
$$

(2)

where $v_{k_l}$ denotes the $l$-th component of the group velocity $\mathbf{v}_k = \nabla \epsilon_k$ of the carriers. The expression in curly brackets in (4) has the perturbation expansion shown in Fig. 1. For $d \to \infty$, momentum conservation at the irreducible vertex part $\Gamma$ becomes unimportant, i.e. the two $\mathbf{k}$ sums for the second and all higher order contributions in Fig. 1 can be performed independently. Since $\mathbf{v}_k$ and $\epsilon_k$ have different parity, these contributions vanish identically [15], and we are left with the simple bubble diagram. Inserting the usual tight-binding expression $\epsilon_k = -2t \sum \cos(k_l a)$, the bubble diagram can be evaluated using standard techniques and leads to the final form

$$
\sigma(\omega) = \sigma_0 \int d\omega' \int d\epsilon A_0(\epsilon) A(\epsilon, \omega') A(\epsilon, \omega' + \omega) \frac{f(\omega') - f(\omega' + \omega)}{\omega}
$$

(3)

for the optical conductivity. Here, $A_0(\epsilon) = 1/\sqrt{4 \pi dt^2 \exp[-\epsilon^2/(4dt^2)]}$ denotes the one-particle density of states for the noninteracting system, $A(\epsilon, \omega)$ the one with $U > 0$, $f(\omega)$ is Fermi’s function and $\sigma_0$ collects all remaining constants and is given by

$$
\sigma_0 = \frac{4d^2 \pi e^2 a^2 t^2}{2\hbar} \frac{N}{V a l} \approx 10^{-2} \ldots 10^{-3} [\mu \Omega cm]^{-1}
$$
for typical values $2\sqrt{\text{dt}} \approx 1\text{eV}$ and $a = O(a_0)$. For convenience we shall choose $4\text{dt}^2 = 1$ in the following.

The only unknown quantity entering into (5) is the one-particle density of states $A(\epsilon, \omega)$ or equivalently the one-particle self energy $\Sigma(k, z) \overset{d=\infty}{\rightarrow} \Sigma(z)$. As mentioned earlier, in $d = \infty$, the task of determining $\Sigma(z)$ reduces to the solution of an effective single impurity Anderson model \[10\] and there exist several reliable methods to handle this problem exactly by e.g. quantum Monte Carlo methods \[10,12\] or approximately within the so called NCA \[14\]. Because the quantum Monte Carlo does not provide the self-energy for real frequencies, the latter approach proves to be more adequate here. We emphasize that the one-particle spectra obtained by the NCA were carefully compared to the exact quantum Monte Carlo results \[13\] and found to be in excellent quantitative agreement over a wide range of model parameters and temperatures. The results presented here can thus be expected to be very close to the exact ones.

In Fig. 2 we show the variation of the one-particle density of states (Fig. 2a) and the optical conductivity (Fig. 2b) for the half-filled case for various values of $U$ calculated at a temperature $\beta = 4$. The DOS suggests a profound change in the qualitative behaviour of the system. Starting from a single central peak at $\mu$ for $U \rightarrow 0$, the characteristic LHB and UHB develop. The broad central peak, still present at intermediate $U$, gradually vanishes and is replaced by a pseudo-gap at $\mu$. This behaviour is reflected in the optical conductivity in Fig. 2b. While for small $U$ only a Drude peak is present, the additional charge excitation peak at $\omega = U$ shows up with increasing $U$. At the same time the weight for $\omega \rightarrow 0$ is drastically reduced. For $U = 5$ we find a situation one would expect for an insulator: Vanishing dc-conductivity and a peak at $\omega = U$ reflecting these induced transitions from the LHB to the UHB. The inset in Fig. 2b gives a logarithmic blow-up of the situation for small $\omega$, clearly showing the reduction of the dc-conductivity by four orders of magnitude as we go from $U = 1$ to $U = 5$.

Away from half filling, one important question is whether the Hubbard model (1) is a
conventional Fermi liquid or not? In Fig. 3 results for the DOS and optical conductivity for some selected temperatures at fixed $U = 4$ and filling $n_e = 0.97$ are shown. As for the DOS (Fig. 3a), we again observe the temperature independent LHB and UHB separated by a pseudo-gap above $\mu$. With decreasing temperature, however, a narrow quasiparticle band develops at $\mu$. This band can be traced to a version of the Kondo-effect in this model and one consequently has to expect a physical behaviour similar to the well studied heavy fermion systems. In fact, the optical conductivity in Fig. 3b shows a strongly temperature dependent Drude peak in addition to the charge excitation peak at $\omega \approx U$. One also clearly sees that the spectral weight built up at $\omega \to 0$ is taken from this peak at $\omega \approx U$. The inset gives again an enlarged view of the situation for $\omega \to 0$.

It is of course interesting to study the temperature dependence of $\sigma(0)$ or $\rho(T) = 1/\sigma(0)$ more closely. If the system were a Fermi-liquid at low temperatures, we should observe $\rho(T) \sim (T/T_0)^2$, where $T_0$ is the effective bandwidth for the quasiparticles. Figure 4 shows the resistivity for $U = 4$ and $n_e = 0.97$ along with the low temperature data versus $T^2$ in the inset. The latter nicely fall onto the curve $\rho(T) = a \cdot (T/T_0)^2$, where $a = O(1)$ and $T_0$ is roughly the width of the quasiparticle peak at $\mu$ in the DOS in Fig. 3a. From this result one clearly has to conjecture that at least for high spatial dimensions the low temperature (paramagnetic) phase of the Hubbard model for fillings $n_e < 1$ is a (possibly heavy) Fermi-liquid. At higher temperatures the resistivity changes from a metallic to a semi-metallic behaviour. This is also consistent with the vanishing of the quasiparticle peak at $\mu$ for high temperatures.

To summarize, we presented characteristic results for the optical conductivity and resistivity of the Hubbard model in $d \to \infty$. The data shown were calculated within an approximate method to solve the impurity Anderson model, which essentially determines the physics of the Hubbard model in this limit. Let us stress that this approximation was shown to very accurate in its domain of applicability \cite{13}. The results at half filling suggest a crossover from a normal metal to an insulator as a function of $U$ with a $U_c \approx 3 \ldots 4$. Further results not presented here \cite{13} show that this scenario does not change qualitatively for lower
temperatures. Off half filling we encounter a Fermi-liquid at low temperatures together with a crossover to a semi-metal at high temperatures. In both cases the optical conductivity reflects the relevant low temperature energy scales of the model, the bare bandwidth $t$ at small $U$ and the Coulomb energy plus possibly a dynamically generated scale $T_0$ for the quasiparticles in the Fermi-liquid for large $U$.

The general behaviour of the two quantities studied here fits at least qualitatively into the picture of the normal state properties of high-$T_c$ superconductors. There are, though, obvious differences, the most important is probably the missing linear low temperature resistivity generally found in the cuprates. One must, however, bear in mind that our results are strictly valid only for $d \rightarrow \infty$ and that especially in 2D dimensional effects will of course be important. For example, one aspect clearly absent in $d \rightarrow \infty$ are spin-fluctuations. As was shown recently [16] the coupling to these degrees of freedom may easily change the power-law in $\rho(T)$. Thus, with a proper account for corrections due to finite dimensions, our results may well be a first step towards the solution of outstanding questions in the field of highly correlated systems.

ACKNOWLEDGMENTS

This research was supported by the National Science Foundation grant number DMR-88357341, the National Science Foundation grant number DMR-9107563, the Ohio State University center of materials research and by the Ohio Supercomputing Center.
REFERENCES

[1] J. Hubbard, Proc. R. Soc. A276, 238(1963); M.C. Gutzwiller, Phys. Rev. Lett. 10, 159(1963); J. Kanamori, Prog. Theor. Phys. 30, 257(1963).

[2] For a review about the theory of the Hubbard model see e.g. D. Vollhardt, Rev. Mod. Phys. 56, 99(1984).

[3] E.H. Lieb and F.Y. Wu, Phys. Rev. Lett. 20, 1445 (1968); H. Frahm and V.E. Korepin, Phys. Rev. B42, 10533(1990); N. Kawakami and S.-K. Yang, Phys. Rev. Lett. 65, 2309(1990).

[4] C.M. Varma, P.B. Littlewood, S. Schmitt-Rink, E. Abrahams and A.E. Ruckenstein, Phys. Rev. Lett. 63, 1996(1989).

[5] P.W. Anderson, Phys. Rev. Lett. 64, 1839(1990); 65 2306(1990).

[6] W. Metzner and D Vollhardt, Phys. Rev. Lett. 62, 324 (1989).

[7] E. Müller-Hartmann, Z. Phys. B 74,507 (1989).

[8] U. Brandt and Ch. Mielsch, Z. Phys. B75, 365(1989); 79, 295(1990).

[9] V. Janiš and D. Vollhardt, Int. J. Mod. Phys. B6, 731(1992).

[10] M. Jarrell, Phys. Rev. Lett. 69, 168(1992).

[11] A. Georges and G. Kotliar, Phys. Rev. B45, 6479(1992); see also the subsequent work of Rosenberg, Zhang, and Kotliar, preprint Feb 1992 and Georges and Krauth, preprint Feb. 1992.

[12] M. Jarrell and Th. Pruschke, accepted for publication to Z. Phys.

[13] Th. Pruschke, D.L. Cox and M. Jarrell; to be published.

[14] H. Keiter and J.C. Kimball, Intern. J. Magnetism 1, 233(1971); Th. Pruschke and N. Grewe, Z. Phys. B 74, 439(1989).
[15] A. Khurana, Phys. Rev. Lett. 64, 1990(1990).

[16] T. Moriya, Y. Takahashi, K. Ueda, J. Phys. Soc. Jpn. 59, 2905(1990).