Numerical Evidence of Luttinger and Fermi liquid behavior
in the 2D-Hubbard Model

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Abstract

The two dimensional Hubbard model with a single spin-up electron interacting with a finite density of spin-down electrons is studied using the quantum Monte Carlo technique, a new conjugate gradient method for the evaluation of the Edwards wavefunction ansatz, and the standard second order perturbation theory. We performed simulations up to 242 sites at $U/t = 4$ reaching the zero temperature properties with no “fermion sign problem” and found a surprisingly good accuracy of the Edwards wavefunction ansatz at low density or low doping. The conjugate gradient method was then applied to system up to 1922 sites and infinite $U$ for the Edwards state. Fermi liquid theory seems to remain stable in 2D for all cases studied with the exception of the half filling case where a “Luttinger like behavior” survives in the Hubbard model, yielding a vanishing quasiparticle weight in the thermodynamic limit.
The anomalous properties found in several High T-c oxides have renewed a considerable attention and an increasing interest for the simplest models which may explain non conventional behavior beyond the Fermi-liquid theory of normal metals and the BCS theory of usual superconductors. The Hubbard model is now the most popular hamiltonian in condensed matter physics and the search for a satisfactory solution in two spatial dimension represents one of the most important challenge in theoretical physics. In one dimension we now have a complete solution, not only for the energy spectrum, but also for asymptotic properties of correlation functions. The physics of the 1D Hubbard model is well described by the Luttinger liquid theory. The Fermi liquid theory is unstable in this case due to divergences in perturbation theory (PT). Such divergences are usually not present in higher dimensionality and a possible anomalous phase in 2D - as suggested by P. W. Anderson - can be explained only within a non perturbative approach.

Historically before the Lieb-Wu exact solution a much simpler case was solved; it is the case when only one particle with spin up interacts with a finite density of spin down electrons. Although this problem is very much simplified and probably far from reality, it already contains the basic features of 1D conductors: the quasiparticle weight vanishes in the thermodynamic limit, and the spectrum consists of holon and spinon elementary excitations.

In this paper we attempt to search for a non Fermi liquid phase in the 2D Hubbard model in this simplified sector. In fact although we do not provide an exact analytical solution, the numerical advantages will be clearly evident in this single spin-flip Hilbert-space of the model.

We thus consider the Hubbard model on a bipartite lattice, where the spin-up and a finite density $\rho = N/L$ of $N$ spin down electrons hop through the $L$ lattice sites with different hopping amplitudes, $t_c$ and $t_d$ respectively. The hamiltonian therefore reads:

$$H = \sum_{R,\tau_\mu} t_c c_R^{\dagger} c_{R+\tau_\mu} + t_d d_R^{\dagger} d_{R+\tau_\mu} + U \sum_R c_R^{\dagger} c_R d_R^{\dagger} d_R$$

where $d (c)$ are fermion operators for spin down (spin up) electrons, $\tau_\mu$ are the 2d nearest
neighbor vectors and \( d (= 2) \) is the spatial dimension.

We are interested in the quasiparticle weight:

\[
Z_p = | < \psi_G | d_p^\dagger | \psi_F > |^2. \tag{2}
\]

where \( | \psi_G > \) is the ground state of \( H \) in the single spin flip subspace and with finite momentum \( p \), and \( | \psi_F > = \prod_{\epsilon_k \leq \epsilon_F} c_k^\dagger | 0 > \) is the non interacting electron sea of spin down electrons, i.e. the ground state of \( H \) without \( d- \)electrons. Such a state is assumed in the following to be a non degenerate, translation invariant closed shell state where \( \epsilon_k = t_c \sum_{\tau} e^{i k \tau} \), and \( \epsilon_F \) is the Fermi energy of the down-spin electrons. \( | \psi_F >\) satisfies these properties only for particular number of electrons, e.g. \( N = 1, 5, 13, \ldots \), covering all possible densities in the thermodynamic limit.

As well known, the quasiparticle weight \( Z_p \) measures the strength of the \( \delta- \)function in the spectral function and is finite in the thermodynamic limit if Landau-Fermi liquid theory is valid. For example in one dimension, where Fermi liquid theory breaks down, \( Z \) vanishes as a power law in the thermodynamic limit , as predicted by the Luttinger liquid theory \( Z \propto N^{-\theta} \). The Hubbard model in the single spin-flip sector is consistent with this general solution and thus represents one of the simplest toy models where Fermi-liquid theory can be tested in higher dimensions.

The hamiltonian \( H \) can be further simplified by tracing out exactly the \( d- \)electron component from the ground state wavefunction. In fact, using translation invariance we can write the ground state \( | \psi_G > \) of total momentum \( p \) in the following form:

\[
| \psi_G > = \frac{1}{\sqrt{L}} \sum_R e^{-ip R} T_R d_O^\dagger | \psi > \tag{3}
\]

where \( | \psi > \) is a wave function depending only on the spin- down electrons, \( T_R \) is the translation operator by a vector \( R \) \( (T_R \ c_{R'} T_{-R} = c_{R+R'} ) \) and \( O \) is the origin of the lattice. Then the following effective hamiltonian \( H' \) for \( | \psi > \) is obtained:

\[
H' = t_c \sum_{R, \tau} c_{R+\tau}^\dagger c_R + t_d \sum_{\tau} e^{-i p \tau} T_{\tau} + U \ c_O^\dagger c_O. \tag{4}
\]
Note that $H'$ is not translation invariant and that the on site Coulomb repulsion $U$ becomes now a simple one-body contribution, i.e. quadratic in the fermion fields. Using Eq. (3) $Z_p$ in Eq. (2) is replaced by the overlap between the $U = 0 \ (|\psi_F >$) and the finite $U$ ground state, at fixed number of electrons: $Z_p = |<\psi_F|\psi >|^2$. Thus the question of Fermi liquid or non Fermi liquid theory in this model is simply related to the stability of the ground state of $H'$ under the local perturbation $U c_O^\dagger c_O$.

Another useful quantity which we will consider in the following is the momentum distribution of the $d-$electron: $n_k = <\psi_G|d_k^\dagger d_k|\psi_G >$. By means of Eq. (3) $n_k$ is related to the expectation value of the $p-k$-momentum projector on the state $|\psi >$: $n_k = <\psi|P_{p-k}|\psi >$, where the projector on the subspace of momentum $Q$ is $P_Q = \frac{1}{L} \sum_R e^{-iQR} T_R$. By inserting in $<\psi|P_{p-k}|\psi >$, a complete set $|\psi_j >$ of translation invariant states containing $|\psi_F >$, it easily follows that:

$$n_p \geq Z_p \quad (5)$$

The previous relation can be viewed as a particular case of the Migdal theorem relating the jump of the momentum distribution at the Fermi surface to the amplitude of the spectral weight. In fact we expect that the inequality (5) turns in an exact equality in the thermodynamic limit.

As it is easy to verify the ground state of the hamiltonian (4) is a free electron Slater determinant in several limiting cases. For $N = 1$-corresponding to the two electron problem for the hamiltonian $H$- there is of course no correlation in $H'$. For $t_d = 0$ the hamiltonian becomes the well known Falikov-Kimball model and the effective hamiltonian $H'$ is free and exactly solvable. The ground state in presence of the local perturbation $U c_O^\dagger c_O$ is orthogonal to the non interacting state, yielding $Z_p \propto N^{-\theta}$ [3]. Finally for $U = 0$ as well as for $t_d \rightarrow \infty$ the free Fermi gas $\psi_F$ is the ground state and $Z_p = 1$.

The above limiting cases are not surprising since only the term proportional to $t_d$–the spin-up kinetic term–is a true many body term in the effective hamiltonian $H'$, all remaining ones being one-body contributions. Moreover this spin up kinetic term is obviously not
extensive in the size of the system and can weakly affect the correlation in the ground state. Based on the previous considerations it is likely that the ground state of $H'$ is always very close to a simple Slater determinant and thus an Hartree-Fock (HF) wavefunction (i.e. the Slater determinant which minimize the expectation value for the energy) may have a very good overlap with the exact ground state of $H'$.

The HF wavefunction of the hamiltonian (1) $|\psi_{EWA}\rangle$ is nothing but the Edwards wavefunction ansatz (EWA), which is exact in 1D for $t_d = t$ and very accurate in energy in the 2D case \[6\]. Nevertheless such an Hartree-Fock wavefunction corresponds ,by Eq.(\[6\]) , to a non trivial correlated state of the Hubbard hamiltonian $H$. It is actually a linear combination of $L$-free electron states, yielding for instance the Bethe-ansatz wavefunction in 1D \[6\].

We have used a well known Quantum Monte Carlo (QMC) technique \[7\] to evaluate the quasiparticle weight $Z_p$ and the momentum distribution $n_p$ in this simple model for $p = 0$ and $t_c = t_d$. The ground state $|\psi_G\rangle$ is filtered out by imaginary time propagation of a given trial wavefunction $|\psi_T\rangle$, $|\psi_G\rangle \propto \lim_{t \to \infty} e^{-tH} |\psi_T\rangle$, after the usual Trotter-Suzuki decomposition of the imaginary time in $P$ slices of length $\Delta \tau = \frac{t}{P} |\psi_T\rangle = |\psi_F\rangle$ in all the present simulations. The unrestricted Hartree-Fock calculations for the EWA and the straightforward second order perturbation theory for $Z_p$ and $n_p$ -coinciding at this order-, are compared with the QMC simulations on finite lattices, $l\sqrt{2} \times l\sqrt{2}$, with periodic boundary conditions tilted by 45 degrees and odd $l$. The convergence in imaginary time is systematically reached within statistical errors in all cases studied. In fact for the Hubbard model in the single spin-flip sector the QMC does not suffer the so called “fermion sign problem”, since in the worst case ($l = 11$) the average sign is approximately 0.6.

In all the QMC simulations I have always found $n_{p=0}$ and $Z_{p=0}$ equals within statistical errors, with an error bar for $n_p$ three times smaller than the one for $Z_p$. $n_p$ is an upper bound for the quasiparticle weight (Eq.\[5\]) but it is always very close to $Z_p$. For instance when $t_d = 0$ or within the EWA approximation $n_0 - Z_0 \leq 10^{-4}$ for all sizes studied. In the following we thus identify the two quantities for the sake of simplicity.
We got very accurate results for the evaluation of the EWA wavefunction using a new conjugate gradients (CG) technique for electronic structure calculations. In order to apply the CG algorithm \cite{8} to the minimization of an energy functional \( E(\{\psi_n\}) = \frac{\langle \psi | H' | \psi \rangle}{\langle \psi | \psi \rangle} \), the orbitals \( \psi_n(k) \) of the Slater determinant \( |\psi> \) have to be orthogonalized from time to time for numerical stability \cite{8}. In doing so one spoils the efficiency of the conjugate directions, and the minimization of the energy becomes slower. This is why the standard CG algorithm with orthogonalization does not improve much the steepest descent scheme, as also discussed in \cite{3}.

In order to solve the previous difficulty we have used the following simple scheme. Since the functional \( E(\{\psi_n\}) \) is invariant for any transformation of the orbitals \( \psi_n \rightarrow \sum_m A_{n,m} \psi_m \) it is possible to choose the \( N \times N \) matrix \( A \) such that the orbitals read: \( \psi_n(k) = \delta_{k,k_n} + u_n(k) \), where \( k_n \) are wavevectors inside the Fermi surface \( \epsilon_{k_n} \leq \epsilon_F \) and the functions \( u_n(k) \) all vanish for \( \epsilon_k \leq \epsilon_F \). The number of independent degrees of freedom is thus \( N(L - N) \), as it should be from general ground. In this way we fix the gauge of the transformations, that leave \( E \) unchanged, and we apply the CG strategy, without orthogonalization requirements. The method is of course not restricted to the plane wave basis for the orbitals \cite{1}. In the largest sizes simulations (\( \approx 2000 \) sites) this novel CG minimization is approximately an order of magnitude more efficient compared to the usual steepest descend method. This factor increases with the size of the system, opening new possibilities for large scale simulations. Further details of this new method will be published elsewhere \cite{1}.

At low density we have studied closed shell systems with the closest density just below and above the value \( \rho = \frac{1}{4} \). This sequence should converge to \( \rho = \frac{1}{4} \) in the thermodynamic limit and should minimize size effects. In Fig. \cite{4} we see that size effects are very important and it is not possible to obtain reasonable conclusions with a small size calculation. The EWA is exact for \( N = 1 \) (smallest size in Fig. \cite{4}) and is a test of our QMC scheme. We note that the results obtained with the EWA are practically indistinguishable from the QMC data, yielding a strong support for the accuracy of the EWA even for relatively large size (up to 242 sites), not accessible by exact diagonalization.
Further evidence for the accuracy of the EWA is given by the explicit calculation of the energy fluctuations $\Delta E^2 = < \psi | H^2 | \psi > - < \psi | H | \psi >^2$ on the EWA $| \psi > = |\psi_{EWA} >$. $\Delta E^2$ vanishes for an exact eigenstate and is given by $U^2 \rho (1 - \rho)$ for the Fermi gas wavefunction $| \psi_F >$. The Edwards wavefunction typically improves this variance by three order of magnitude compared to the Fermi gas wavefunction which still is very good for this small positive $U$ value. As shown in Fig. 1 the behavior of the QMC data up to $l = 11$ and the EWA data for larger systems up to $l = 31$ are very similar to the PT, which is finite for $d = 2$ and $\rho \neq \frac{1}{2}$ . Furthermore EWA and QMC data are always well above the PT results, strongly suggesting that $Z_p$ should be finite in the exact calculation as well as for larger $U$ ($U = \infty$ is shown in Fig. 1). Similar scenario appears also evident for negative $U$ (Fig. 2), corresponding by the particle - hole transformation to positive $U$ at density $1 - \rho = \frac{3}{4}$, i.e. the low doping region. However in this case the PT results for $Z_p$ are larger than the QMC and EWA data and the conclusion of a finite $Z_p$, although quite likely, is less clear. Note also that for infinite $U$, $Z_p$ seems to drop at the largest sizes.

At half filling $L/2 = N = l^2$ the $U = 0$ ground state is a non-degenerate closed shell. The Fermi surface is a square and is commensurate with the finite mesh in the Brillouin zone, leading to size effects very smooth and well controlled. In Fig. 3 we show Quantum Monte Carlo results as a function of $\Delta \tau^2$. The $\Delta \tau^2 \to 0$ limit should be considered a formally exact and unbiased property of the ground state for long enough $t$. The results obtained with the EWA are systematically larger than the QMC data, except for small sizes.

In this case the second order PT is logarithmically divergent due to the nesting of the Fermi surface: $\ln Z_{p=0} = -U^2 0.00335002 \ln(L) + O(U^4)$. As in 1D this kind of divergence suggests a power law decaying for $Z_p \propto N^{-\theta}$. In fact as shown in Fig. 3(b) the ln-ln plot appears linear for $\ln(L) \to \infty$ both for the PT data ($\theta_{PT} = 0.0536002$) and for the EWA ones ($\theta_{EWA} = 0.028$). The QMC data lie in between the two straight lines giving a strong evidence that $Z_p$ eventually vanishes as a power law wit $\theta \sim 0.04$. This is maybe one of the first example of Luttinger-like behavior in a 2D system and represents the central result of this paper. It is also interesting to note that the Luttinger liquid exponent for $U = \infty$ is very
close to $\theta = \frac{1}{8}$ for the EWA data, exponent well known in 1D where it can be determined exactly \[ (\ref{10},\ref{11}) \].

In conclusion we have presented an accurate and well controlled size scaling of the quasiparticle weight in a numerically tractable sector of the 2D Hubbard model. We have used QMC and a new conjugate gradient algorithm for the evaluation of the EWA. This ansatz turns out to be an almost exact approximation in most cases for $U = |4t|$.

The quasiparticle weight $Z_p$ looks always finite with the noticeable exception of $\rho = \frac{1}{2}$, where the nesting of the Fermi surface leads to a power law decaying $Z_p$, as well as to a logarithmically divergent PT. At low doping and large $U$ a non perturbative break-down of Fermi liquid theory is not inconsistent with our data, and further study is needed to clarify this issue.

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FIGURES

FIG. 1. (a) QMC data (empty dots) vs. EWA ones (full squares) for $U = 4t_c$ and $t_c = t_d$. The continuous line (upper $\rho < 1/4$) connects EWA data for $N = 1, 9, 21, 37$, the lower curve (dashed $\rho > 1/4$) for $N = 5, 13, 25, 45, 61$. The QMC data are converged in imaginary time for $t = l + 4$ with $l = 3, 5, 7, 9, 11$ from left to right. The $\Delta \tau$ correction was estimated for $l = 3, 5, 7$ with several points (see Fig. 3). (b) EWA data for $U = 4t_c$ (continuous line) and $U = \infty$ (long dashed line) up to $l = 31$ compared with second order PT results (dashed line). The arrow indicates the infinite size PT result. The lines are guides to the eye.

FIG. 2. same as Fig. 1 for negative $U$. The QMC data refers to $l = 3, 5, 7, 9$. Similar considerations apply for the $\Delta \tau$ corrections and the imaginary time error was negligible for $t = l + 6$.

FIG. 3. (a) logarithmic plot of the quasiparticle weight. The empty dots are QMC data after extrapolation to $\Delta \tau \to 0$. The continuous line and the long dashed line connect EWA data for $U = 4t_c$ (full dots) and $U = \infty$ (full squares) respectively. The number of electrons was fixed to $N = l^2$ for $l = 3, 5, \ldots, 23$. The PT data (full triangles) were calculated up to $l = 53$ (not shown in the picture) and the dashed line is the exact slope in the thermodynamic limit. (b) QMC data as a function of $\Delta \tau^2$ for $U = 4t_c$ and the imaginary time $t = l + 6$, large enough to have converged results. The continuous lines are least square fit of the data and the dashed line ($l = 9$) has a slope estimated from the smaller sizes. The arrows indicate the EWA values for $l = 3, 5, 7, 9$ from top to bottom figure respectively.