NUMERICAl STUDY OF THE 2D HUBBARD MODEL AT HALF FILLING

S. Sorella, A. Parola, M. Parrinello, and E. Tosatti

Scuola Internazionale Superiore di Studi Avanzati

Strada Costiera 11, I-34014 Trieste - Italy

ABSTRACT

The ground state of the 2D (square lattice) finite-size Hubbard model is studied at half filling with a newly developed Quantum Monte Carlo method. We have studied square cells from 18 to 242 sites for $U = 3$ with high statistical accuracy to perform a reliable size scaling analysis. The results confirm that the system is an antiferromagnetic insulator. The finite size scaling results are discussed in detail, focusing on the behaviour of magnetization, and most particularly of momentum distribution.

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The Hubbard model is currently a subject of intensive study because of its possible relevance for the physics of Hi-T_c superconductors[1]. The Hubbard model is described by the hamiltonian

$$\hat{H} = \hat{K} + \hat{V} \tag{1}$$

where $\hat{K}$ is the kinetic term which allows hopping of electrons between nearest neighbour sites

$$\hat{K} = -t \sum_{\langle ij\rangle,\alpha} c^{+}_{i\alpha} c_{j\alpha} \tag{2}$$

and V represents the on site coulomb repulsion:

$$\hat{V} = U \sum_{i} c^{+}_{i\uparrow} c_{i\uparrow} c^{+}_{i\downarrow} c_{i\downarrow} \tag{3}$$

Here $\sum_{\langle ij\rangle}$ indicates nearest neighbours sum, the indices run over the N lattice sites, $c^{+}_{i\alpha}$ ($c_{i\alpha}$) are the usual creation (annihilation) operators at site i with spin α, and $U > 0$.

Despite its apparent simplicity the Hubbard model embodies all the difficulties of a truly interacting system. Without interaction ($U = 0$) one obtains a pure band behaviour typical of the kinetic term $\hat{K}$. In the atomic limit ($t = 0$) the particles are localized. So the Hubbard Hamiltonian describes a system which allows for both these limits. Of course the intermediate regime ($t \sim U$) is of particular interest, as in this range of parameters the competition between band effects and localization due to the correlation is most important. So far only the one–dimensional case has been solved exactly [2–4]. For higher dimensions mostly approximate results are available (besides a few exact results within perturbation theory[5,6]). Of particular interest are also exact results about the limit $D \to \infty$[7,8], where D is the physical dimensionality.

A major development in the understanding the physics of the Hubbard model has been provided by the use of computer simulation techniques. For fermions, a major difficulty of Quantum Monte Carlo (QMC) methods is the so called "fermion sign problem"[9], which, when present, does not permit the definition of a positive definite probability function. Hirsch [10,11] has shown, using a Hubbard Stratonovich formulation, that it is possible to study the half filled Hubbard model without any "fermion sign problem", thanks to charge conjugation symmetry. Some of his results may be summarized as follows.

The system is antiferromagnetic and a good mean field starting point is band antiferromagnetism, i.e., Hartree Fock (HF) spin density wave.

The Hartree Fock spin density wave (SDW) theory of the Hubbard model predicts a value of the staggered magnetization m that in $D = 2$ for small U behaves as:

$$m_{HF} \propto \frac{t}{U} e^{-2\pi\sqrt{\frac{t}{U}}} \tag{4}$$

An important point is that within the HF theory there is a very simple relation between the gap of the charged excitation Δ_{ch} and the value of the magnetization

$$\Delta_{ch} = Um \tag{5}$$

This simple relation is expected to remain approximately valid even for the correlated system.

For the 2D half filled Hubbard model Hirsch found[10,11] in fact that the value of the staggered magnetization at a given U can be obtained by using the HF result and correcting it only by a factor α independent of U

$$m = \alpha\, m_{HF}. \tag{6}$$

For $U \to \infty$ the Hubbard model becomes a Heisenberg model and the value of m for this model is quite well established ($m = 0.60$). Using this result together with the assumption (6) the HF results can be scaled by a factor $\alpha = .60$ in the intermediate regime as well. In summary, according to Hirsch, the physical properties of the half filled model can be easily understood by a simple mean field spin density wave picture, corrected only for spin–wave fluctuations.

We present here new numerical work on this subject, using the newly developed technique presented in previous work[12,13]. At half filling, as shown in [14] instead of the imaginary time functional ($\beta = i\,t$):

$$Q = \int d\mu_\sigma \;\; < \psi_T U_\sigma(\beta, 0) \psi_T >, \tag{7}$$

obtained from a straightforward application of the Hubbard Stratonovich transformation, one can use a more convenient functional

$$Q_N(\beta) = \int d\mu_\sigma \; \| U_\sigma | \psi_T > \| \tag{8}$$

In the same notation as in Ref.(13) $U_\sigma(\beta,0)$ is the imaginary time evolution operator, containing the Hubbard Stratonovich random fields $\{\sigma\}$ and ψ_T is a trial determinant wavefunction.

The quantity

$$E_N = \lim_{\beta\to\infty} -\frac{1}{\beta} \ln Q_N^\beta(\psi_T) \tag{9}$$

is exactly the ground state energy for $\beta \to \infty$ and for any trial wavefunction non orthogonal to the half filled ground state. Hence, by the Hellmann–Feynman theorem, ground state expectation values of operators $< \psi_0 \hat{O} \psi_0 >$ can be calculated by differentiating the ground state energy of the Hamiltonian $\hat{H}$ in presence of the perturbation $\lambda\hat{O}$ with respect to λ. Then we get a well defined estimator of any given operator $\hat{O}$

$$< \psi_0 O \psi_0 > = \lim_{\beta\to\infty} < E_0(\sigma) >_N^\beta \tag{10}$$

where the subscript N denotes average over Q_N, and the estimator $E_0(\sigma)$ is:

$$E_0(\sigma) = \frac{\partial}{\partial\lambda}\bigg|_{\lambda=0} -\frac{1}{\beta}\left(\ln \|U_\sigma^\lambda\|\right). \tag{11}$$

Here U_σ^λ is a new imaginary time propagation operator obtained by adding the perturbation $\lambda\hat{O}$ to the kinetic term. If at half filling ψ_T is chosen to be invariant under the charge conjugation transformation it is also true that average quantities (10) converge to the desired ground state expectation value, since, as mentioned in this case there are no fermionic sign problems.

Using numerical methods based on finite systems calculations the staggered magnetization m can be evaluated by studying the real space spin–spin correlation function $C(\mathbf{r})$ for clusters of increasing size $L \times L$

$$m = \lim_{L\to\infty} \sqrt{3\,C\left(\frac{L}{2},\frac{L}{2}\right)} \tag{12}$$

or from the Fourier transform $S(q)$ of the spin–spin correlation function $C(\mathbf{r})$

$$m = \lim_{L\to\infty} \sqrt{\frac{3S(\pi,\pi)}{L^2}} \tag{13}$$

where C in our units is defined as:

$$C(\mathbf{r}) = \frac{4}{3} < \underline{\mathbf{S}}_{\mathbf{r}'} \cdot \underline{\mathbf{S}}_{\mathbf{r}'+\underline{\mathbf{r}}} > \qquad (14)$$

and the factor $\frac{4}{3}$ is used to match our convention with the usual definition. In fact one often uses [10,11,15] a spin correlation function $\zeta(r) = < m_{r'} m_{r'+r} >$ where only local magnetic operators along the z–axis appear. The two definitions are equivalent for a singlet ground state. In our previous work[13] we had used the latter. Here, instead we prefer the symmetric expression (14) to reduce statistical errors.

For a finite size scaling estimation of m by means of eqs.(12,13) it is useful to have a guess about the finite size corrections on the mentioned quantity. This is indeed possible because, according to spin-wave theory, the finite size corrections to the staggered magnetization are expected[15] to vanish as L^{-1}.

In order to perform an accurate finite size scaling of the 2D Hubbard model we restrict our simulations to the particular value $U = 3$. Moreover we work with tilted lattices, as discussed by Oitmaa and Betts[16], rotated by 45^0 with respect to the normal coordinate axis. This geometry has the property that $l\sqrt{2} \times l\sqrt{2}$ (l odd) unit cell yields a closed **k**–space shell, i.e. no degeneracy, at half filling. The number of sites was fixed $N = 2l^2$ where l is an odd integer.

We choose for this simulation a discrete Trotter time $\Delta\tau = .08$ and $\Delta\tau = .16$ as a test for the convergence, while the Langevin dynamic equations were discretized[12] with $\Delta s = \frac{\sqrt{2}}{10}$. The last choice has been checked against systematic errors, that for all quantities studied, turn out to be negligible when compared with the statistical errors. A careful analysis has been performed for the convergence in the imaginary time β. For each size we made several runs with different temperatures until convergence has been reached within statistical error.

In fig.1 we plot the quantity $C(\frac{L}{2}, \frac{L}{2})$ and also $\frac{S(\pi,\pi)}{L^2}$. The data fit quite well a quadratic extrapolation in $\frac{1}{L}$, and this indicates an important size dependence of these quantities on top of the spin–wave behaviour L^{-1}. After extrapolation, which is fairly consistent for both measured quantities, we obtain a finite value of the staggered magnetization in the thermodynamic limit (see eqs.12,13)

$$m = .24 \pm .02 \qquad for\ U = 3 \qquad (15)$$

The corresponding SDW value is .58. The value (15) is somewhat lower than the corrected HF theory described before (see eq.6) which would give $m = .35$. Hence spin density wave HF theory, even corrected with the empirical spin wave factor α, is not very accurate. A possible mechanism in originating this decrease of magnetization is associated with a finite charge gap Δ_{ch} for finite U. We believe that quantum charge fluctuations–somewhat similar to doping– cause a reduction of this gap from its HF value. In view of the qualitative connection (5), this may cause the further reduction of m.

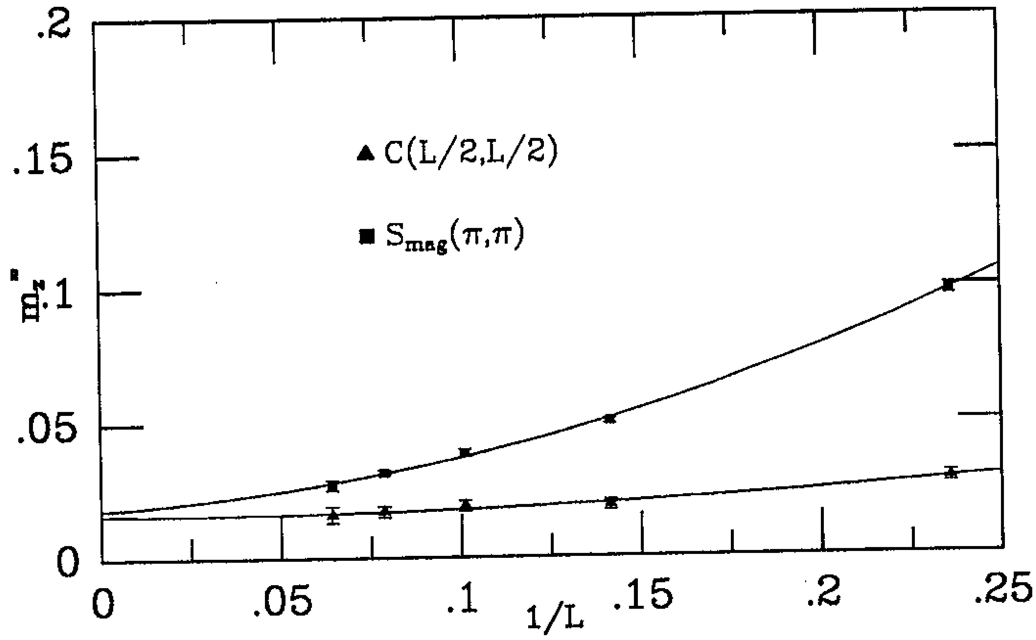

Figure 1. A plot of $\frac{S(\pi,\pi)}{L^2}$ (squares) and $C(L/2,L/2)$ (triangles) against L^{-1} for the 2D Half filled Hubbard model for U=3. The intercept is equal to $m_z^2 = m^2/3$ where m is the value of the staggered magnetization. The curves are quadratic fits of the data.

This close connection between spin–related and charge–related properties suggests the necessity of studying the latter, which seems largely unexplored in the 2D Hubbard model. As a first step, we have performed a detailed size scaling analysis of the momentum distribution function:

$$n_k = < \sum_{\alpha} c^{\dagger}_{\alpha,k} c_{\alpha,k} > . \qquad (16)$$

The metallic or non metallic properties of the ground state are, as is well known, directly related to the presence or the absence of a Fermi jump of n_k in the thermodynamic limit. For this purpose we have used a special analysis of data which we briefly describe below and that can be obviously extended even away from half filling or to higher dimensionality. For reasons of simplicity, we neglect here the further complication arising from the fact that our cells are rotated.

As well known, the resolution in **k** space increases very slowly with the size of the system and it is difficult in 2D or in higher dimensions to reach a reasonable size so as to distinguish whether a Fermi surface is really defined for the infinite system. Instead of considering directly the momentum distribution we find it convenient to consider the related quantity:

$$n_\epsilon = \frac{\int \frac{d^2k}{(2\pi)^2} n_k \, \delta\left(\epsilon(k) - \epsilon\right)}{\int \frac{d^2k}{(2\pi)^2} \delta\left(\epsilon(k) - \epsilon\right)} \tag{17}$$

where $\epsilon(k) = -2(\cos k_x + \cos k_y)$ is the non–interacting electron kinetic energy. For a finite system all the vectors of the Brillouin zone can be divided into different groups with a defined $\epsilon(k) = \epsilon$ (see fig.2). For each group we calculate the average value of the momentum distribution and represent it as a function of ϵ. It is clear that for infinite size this function can be obtained by a surface integral over surfaces $S_\epsilon = \{k \,|\, \epsilon(k) = \epsilon\}$ for $-4 \leq \epsilon \leq 4$ as in (17).

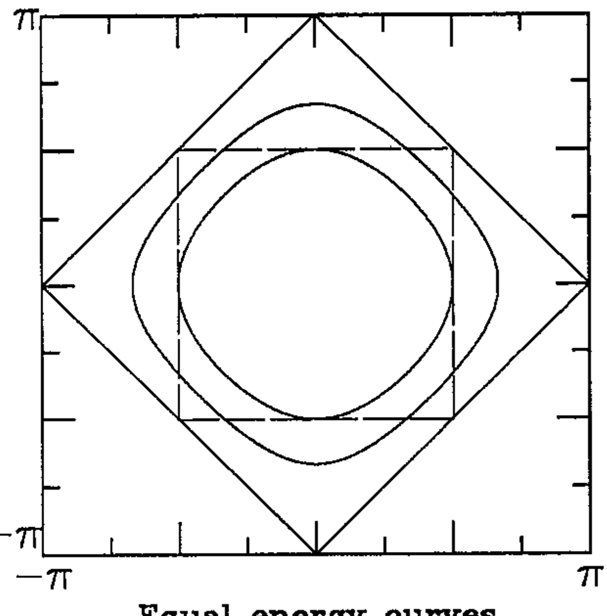

Figure 2. Locus of k-points S_ϵ (continuous lines) with equal kinetic energy for a two-dimensional Hubbard model with nearest-neighbour hopping only. $\epsilon = -2, -1, 0$ starting from the inner surface. The dashed line represents an idealized Fermi surface at an arbitrary filling.

A picture of these surfaces as a function ϵ is plotted in fig.2. An illustrative example

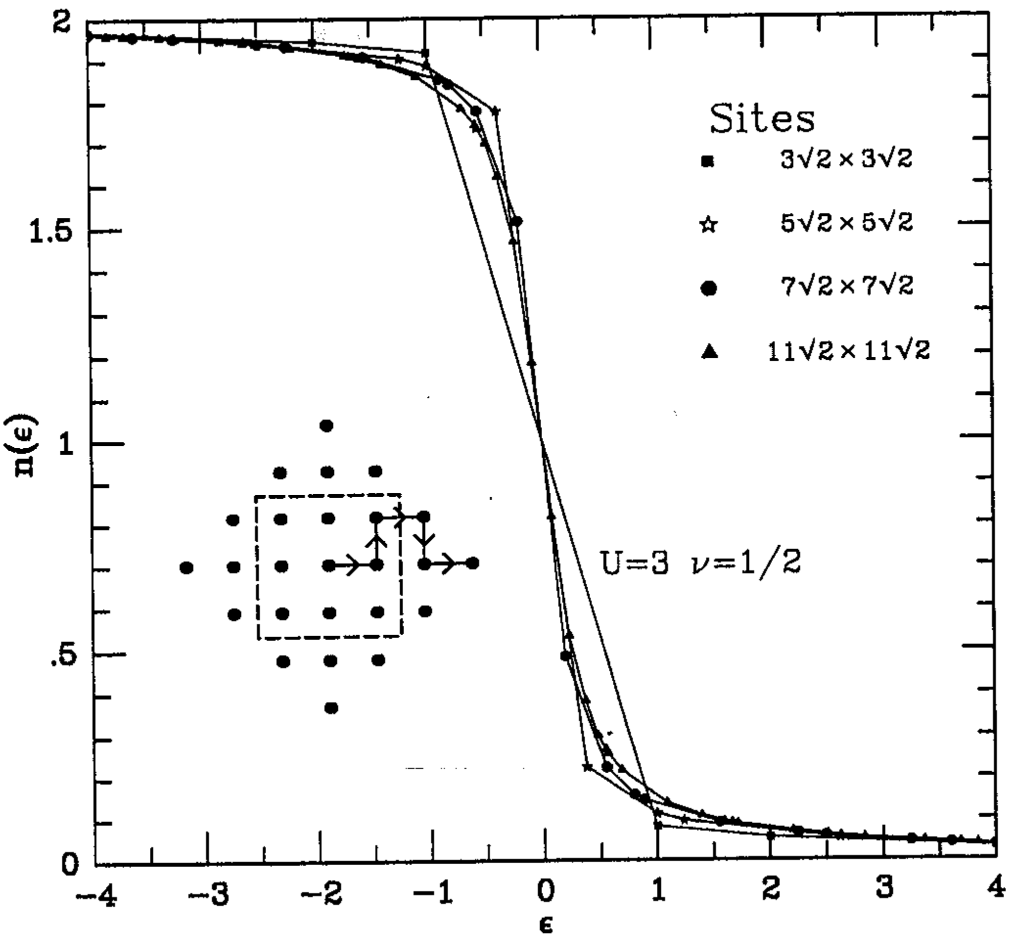

Figure 3. A plot of $n(\epsilon)$ for different sizes for a 2D Hubbard model at half filling. In the particular case $3\sqrt{2}\times3\sqrt{2}$, the k–points involved are shown in the inset, where the dashed line is the $\rho=1$ $U=0$ ideal Fermi surface.

of this function n_ϵ is given by the SDW results where the solution is explicit and simple[17]:

$$n_\epsilon = 1 - \frac{\epsilon}{\sqrt{\epsilon^2 + (\frac{\Delta_{ch}}{2})^2}} \tag{18}$$

Thus, within HF theory n_ϵ is a smooth function of ϵ everywhere including the Fermi energy $\epsilon = 0$, thus indicating the disappearance of the Fermi surface. In fact in that case n_k is easily related to n_ϵ:

$$n_k = n_{\epsilon(k)} \tag{19}$$

The derivative γ of n_ϵ at the Fermi energy is finite and is simply related to the SDW gap Δ_{ch}:

$$\gamma = -\frac{\partial n_\epsilon}{\partial \epsilon} = \frac{2}{\Delta_{ch}^{SDW}} \tag{20}$$

By doping the system, n_ϵ vanishes in a finite range of energy $|\epsilon| \leq |\epsilon_F|$, thus showing the same discontinuity of n_k at the Fermi surface.

More generally, without restricting ourselves to mean field theory, if n_k has a Fermi surface that coincides with one of the possible surfaces S_ϵ for (say) $\epsilon = \epsilon_F$, as it is the case in the previous example, the function $n(\epsilon)$ has a jump in the thermodynamic limit. On the other hand if by increasing ϵ the surfaces S_ϵ touch the Fermi surface only in some points, as it is the case for the dashed surface shown in fig.2, n_ϵ is discontinuous only in its first derivative. In this way, by studying the property of this function for increasing size systems, it is possible to study the appearance of a Fermi surface with a much better resolution $\left(\propto \frac{1}{size}\right)$, with respect to a direct analysis of the momentum distribution in k-space. In fact in the interval $-4 \leq \epsilon \leq 4$ the number of possible values of the discrete energies ϵ is proportional to the finite size of the system.

We plot in fig.3 the function n_ϵ for all different sizes studied. The picture shows that this quantity, depends smoothly on size and does not appear to be singular for any value of ϵ, in agreement with a absence of a Fermi surface, as expected for the antiferromagnetic insulator.

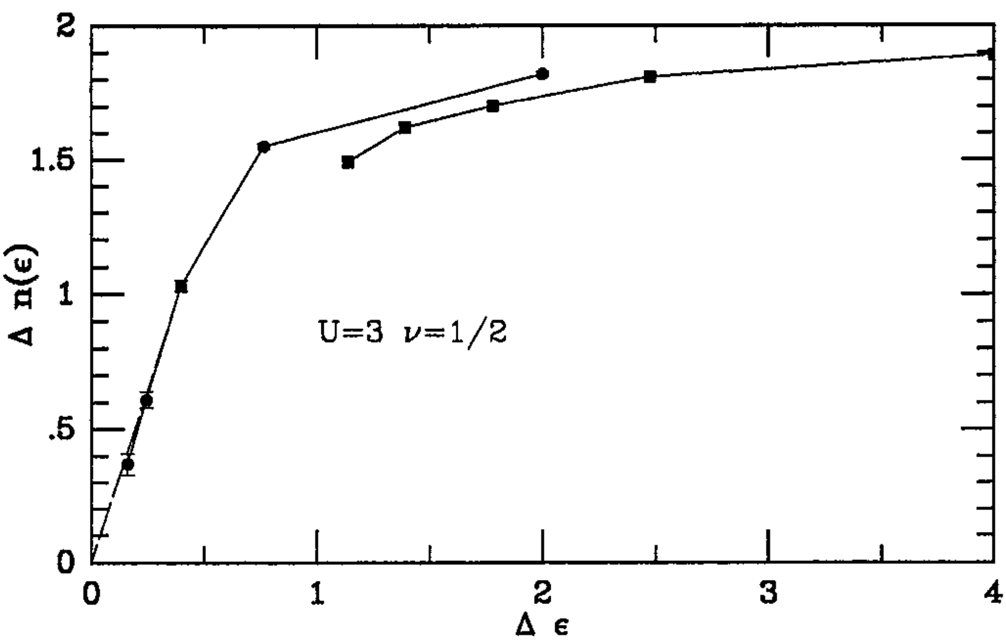

Figure 4. Plot of the maximum jump (full dots) of the function $n(\epsilon)$ described in the text as a function of the finite size resolution in energy for a 2D Half filled Hubbard model. The squares indicates the plot of the jump of n_k in the (1,0) direction as a function of the corresponding difference of kinetic energy for the chosen k values.

In order to describe systematically this property we consider, for a finite system–size L the finite difference $n(-\epsilon_L) - n(+\epsilon_L)$ of the function $n(\epsilon)$ in the two symmetric values of the discrete energies $\pm\epsilon_L$ closest to 0 (the "Fermi jump"). We plot in fig.4 this quantity as a function of the finite energy resolution $2\epsilon_L$ and we see that the finite size Fermi jump seems to approach zero in a linear fashion for $L^2 > 78$. This again indicates that that the sharp nested Fermi surface occurring at $U = 0$ disappears for large enough size due to the interaction. In the same picture we also show for comparison the size dependence of the jump of n_k in the (1,0) direction. This plot demonstrates directly that the finite size scaling of n_k itself would not be meaningful without reaching much larger sizes. This is in fact the reason why we preferred to study the possible singularities of $n(\epsilon)$ in eq.(17).

Moreover this size scaling analysis shows a finite slope γ of n_ϵ for $\epsilon = 0$ (see fig.4). As discussed before the simple HF theory (eq.20) would yield $\gamma = \frac{2}{\Delta_{ch}^{SDW}}$. Using the values shown in fig.4 we can estimate the value of this slope , which is

$$\gamma \simeq 2.6. \tag{21}$$

This result can be compared with the HF value $\gamma = \frac{2}{\Delta_{ch}^{SDW}} \simeq 1.2$ and suggests, in view of eq.(20), a very strong reduction of the charge gap due to quantum charge fluctuations.

We may compare this value (21) with the one obtained by the simple relation $\Delta_{ch} = Um$, using the calculated value of $m = .24$ and, naively, identifying γ with $\frac{2}{\Delta_{ch}}$ (see eq.20). This gives

$$\gamma \simeq 2.8 \tag{22}$$

in fair agreement with the more accurate result (21). This in turns shows that the "corrected mean field theory" gives reasonably quantitative accuracy in this case.

In summary we have described QMC results confirming that the half filled Hubbard model on a square lattice is an antiferromagnetic insulator. The main new results concern 1) accurate finite size scaling for the magnetism, which turns out to be, for $U = 3$, more like $0.4\frac{\Delta_{ch}^{SDW}}{U}$ that $0.6\frac{\Delta_{ch}^{SDW}}{U}$ as expected for $U = \infty$; 2) a study of the momentum distribution, and of the jump at the Fermi level, which is shown to scale to zero, as appropriate for an insulator; 3) the effective (renormalized) charge gap Δ_{ch}, which for $U = 3$ is $\sim \frac{1}{4}$ of its Hartree–Fock value Δ_{ch}^{SDW}.

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