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NUMERICAL SIMULATION OF THE 1D AND 2D HUBBARD MODELS: FERMI LIQUID BEHAVIOR AND ITS BREAKDOWN*

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ABSTRACT

The ground state of the 1D and of the 2D (square lattice) finite-size Hubbard model is investigated for variable filling using a novel quantum simulation method. We have studied up to 256 sites for both 1D and 2D. Away from half filling the 2D antiferromagnetic order is initially destroyed, albeit without any clear sign of a Fermi liquid behaviour. A metallic jump in $n(\mathbf{k})$ appears only very far from half filling. In the 1D case, by contrast, a Fermi liquid-like jump in $n(\mathbf{k})$ is obtained even very close to half filling.

The physical properties of the Hubbard model are of extreme current interest also because of its possible relevance for understanding the mechanisms responsible for high T_c superconductivity. The standard Hubbard hamiltonian reads:

$$H = -\sum_{<ij>,\sigma} c\dagger_{i\sigma} c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow},$$

where $< ij >$ indicates that the sum is over couples of nearest neighbors, σ are spin variables ($\sigma = \uparrow$ or $\downarrow$), $c\dagger$'s and n's are fermionic creation and density operators respectively, and the hopping parameter t is taken as the energy unit. Despite the simplicity of the model and three decades of theoretical efforts[1,2], the corresponding phase diagram is still largely unexplored.

In 1D, the exact Lieb-Wu solution is available[3], which provides (for any finite size as well as the infinite size) the ground state energy as a function of U and of the filling $\nu = \frac{N}{N_a}$, where N_a is the number of lattice sites, and N is the number of electrons. In particular, the ground state at half filling ($\nu = 1$, 1 particle per site) is well known to be an antiferromagnetic (AF) insulator without any long range order for all value of U, while for $\nu \neq 1$ the system is a conductor for any U. In principle, the ground state wavefunction is provided by the Lieb-Wu treatment; however it depends on an unmanageable number of parameters, so that the precise nature of the state and of its correlations is not yet clear.

In 2D, the situation is even more uncertain. It is generally believed that antiferromagnetic long-range order prevails, although marginally, for $\nu = 1$ and that it disappears for $\nu \neq 1$, but the nature of the resulting state is at present controversial. In particular, according to Anderson, a superconducting RVB phase should appear in some region of doping δ ($\delta = 1 - \nu$) as a result of large fluctuations in the number of singlet pairs made possible by the presence of holes[4]. Numerical simulations by Hirsch have failed to detect any other significant feature than the breakdown of antiferromagnetism away from $\delta = 0$[5,6]. In particular Hirsch's work seems to suggest the existence of an ordinary paramagnetic metallic phase as soon as $\nu \neq 1$. However, existing simulations of the ground state of interacting fermions are affected by a number uncertainties due to *i)* small system size, *ii)* non zero temperature making extrapolation to the ground state problematic, and *iii)* non positiveness of the statistical weight.

We have performed numerical simulations using a newly developed technique which seems capable of dealing with the above difficulties. We present here some very preliminary results for the ground state properties of the 1D and 2D (square lattice)

Hubbard models, covering just a few values of U and δ. Our main results are the following: *i)* in 2D, the $\delta = 0$ ground sate is an ordered antiferromagnetic insulator with a smooth momentum distribution $n(\mathbf{k}) = \sum_\sigma < c\dagger_{k\sigma} c_{k\sigma} >$; *ii)* for moderate doping, the long range antiferromagnetism is destroyed, but the momentum distribution seems to retain an insulating character; *iii)* for very large doping, a sharp jump in $n(\mathbf{k})$ signals the transition to a normal Fermi liquid; *iv)* in 1D, by contrast, even a small amount of doping gives rise to a large jump in the momentum distribution which indicates that, at least within the resolution due to the finiteness of our samples, the insulating character of the ground state is destroyed.

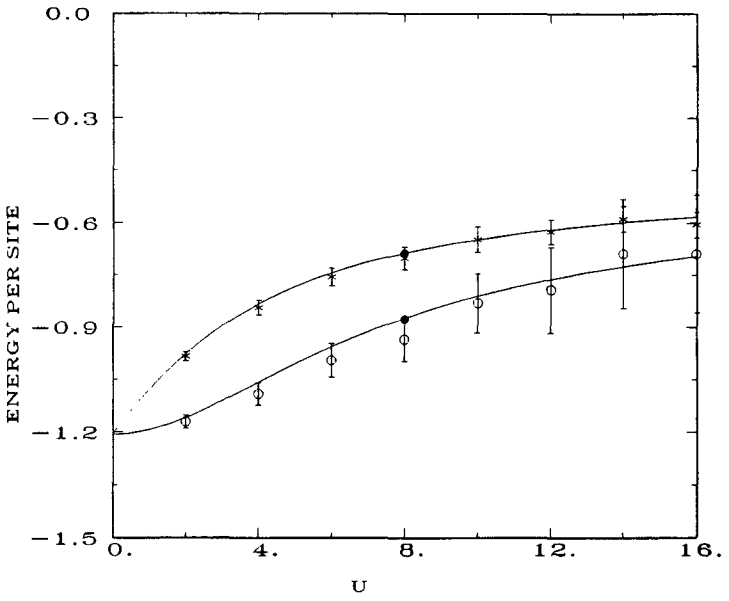

Figure 1. Total energies (upper curve) and kinetic energies (lower curve) for the 8 site 1D Hubbard model, for $\nu = \frac{6}{8}$, as a function of U. The continuous line indicates the exact results obtained by the Lieb and Wu's method. The full dots at U=8 indicate the results obtained with a more precise simulation (see text). Here T=15 is used.

In our scheme, the ground-state properties are obtained by filtering out excited states from a trial Slater determinant wavefunction which is propagated up to a large imaginary time T. The propagation is discretized according to the rule: $U\Delta T \sim \frac{1}{4}$, so that the total number of time slices is $N_T \sim 4UT$. The imaginary time propagator is then converted into a superposition of single-particle propagators by means of the Hubbard-Stratonovich (HS) transformation[7]. The resulting functional integral is evaluated using a statistical-mechanical technique based on Langevin dynamics[8]. The number of steps used to integrate the Langevin equations will be hereafter indicated by

N_S and should not be confused with N_T. The procedure has been successfully tested against exact results for the 8 site 1D system for $\nu = \frac{6}{8}$, where our values for the total and kinetic energies coincide to high accuracy with the results obtained by solving the discrete Lieb-Wu equations. The accuracy can be further sistematically improved by increasing the simulation time. Some typical results from this test are shown in Fig. 1. In this simulation we have used T=15 and the number of Langevin steps was typically $N_s \sim 100$. In order to show how the results can be systematically improved increasing N_S we have performed, in the particular case of $U = 8$, a simulation with $N_s \sim 2500$ Langevin steps. The corresponding results are indicated by the full dots, where the error is smaller than the dimension of the dot. More generally in this as well as in later results the error bars are mainly due to our finite number of Langevin steps N_S rather than to the finite number of time slices N_T.

The full technical details of our method, as well as further tests, will be presented elsewhere[9]. For the time being, we note that the statistical weight resulting from straightforward application of the HS transformation is not always positive definite. In our approach this problem can be handled by evolving the fictitious classical fields and their Langevin equations with a different weight which is always positive definite and yet leads, under numerically controlled conditions, to an identical distribution for $T \to \infty$ (i.e. the ground state)[9].

In Fig. 2 we report our calculated total energy for the 2D 8×8 half-filled (ν=1) Hubbard model as a function of U. The results of a previous Monte Carlo simulation by Hirsch[5] and that of the Hartree-Fock antiferromagnetic state are also shown for comparison. Our results are well within the error bars of previous simulations. However the accuracy of the present method is significantly higher because we approach the ground state without the need for any extrapolation from finite temperature.

In Fig. 3 we show the momentum distribution $n(\mathbf{k})$ of the half-filled ($\nu = 1$) 16×16 lattice for $U = 0.5$ and $U = 4$. The Fermi surface is smeared out in both cases, although very little so for $U = 0.5$. Further evidence that the insulating character is present even at $U = 0.5$ is provided also by the direct evaluation of the single-particle gap $\mu_+ - \mu_-$ (in the Lieb-Wu notation) which is 0.2 ± 0.05. It seems likely that the insulating antiferromagnetic behavior should continue all the way down to $U \to 0$.

In Fig. 4 we display the spin-spin correlation function $\zeta(\mathbf{r}_i - \mathbf{r}_j) = < s^z(\mathbf{r}_i) s^z(\mathbf{r}_j) >$ for the same systems of Fig. 3, clearly exhibiting long-range antiferromagnetism. The staggered magnetization –which would be 1 for the ideal, fully aligned, AF state– is

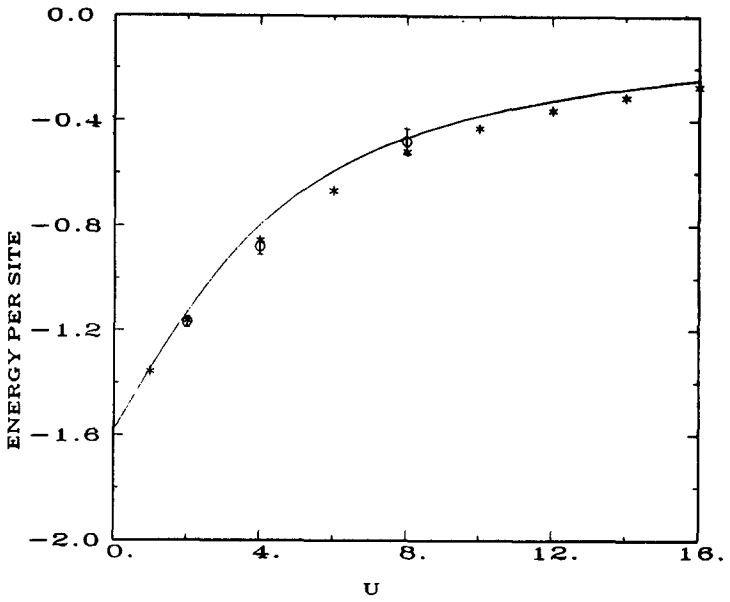

Figure 2. Total energy of the half filled 2D 8×8 Hubbard model as a function of U. Stars indicate our results where the error bars are smaller than the dimension of the symbols; circles indicate results by Hirsch; the continuous line represents the antiferromagnetic Hartree-Fock energy.The results are generally well converged for $T < 20$

approximately 0.37 for $U = 4$ (HF value 0.7) and 0.14 for $U = 0.5$ (HF value 0.15). The antiferromagnetic order is likely to extend over all values of U. Therefore in 2D the metal-insulator transition at $\nu = 1$ seems to occur only for $U = 0$, similarly to the 1D case.

The 2D antiferromagnetic order is readily destroyed by doping. In Fig. 5 we display the spin-spin correlation function ζ in the 16×16 lattice at $U = 4$ for $\nu = \frac{226}{256}$ ($\delta = 12\%$) and for $\nu = \frac{74}{256}$ ($\delta = 71\%$). These results have been obtained using a paramagnetic trial wavefunction. The same results are also recovered starting from an antiferromagnetic wavefunction. However in this case a longer Langevin simulation is needed to reach equilibrium and melt the magnetic order.

The results of Fig. 5 confirm the suggestion by Hirsch that away from $\nu = 1$ the magnetic order is destroyed in the 2D Hubbard model. The question whether spin correlations in this system decay exponentially or as a power law is however difficult to answer within the present numerical accuracy. In fact, the corresponding spin-spin correlations for the $U = 0$ Fermi-liquid look quite similar.

In order to test the further conjecture that the disappearance of magnetic order signals the onset of simple paramagnetic metallic behavior, we have measured

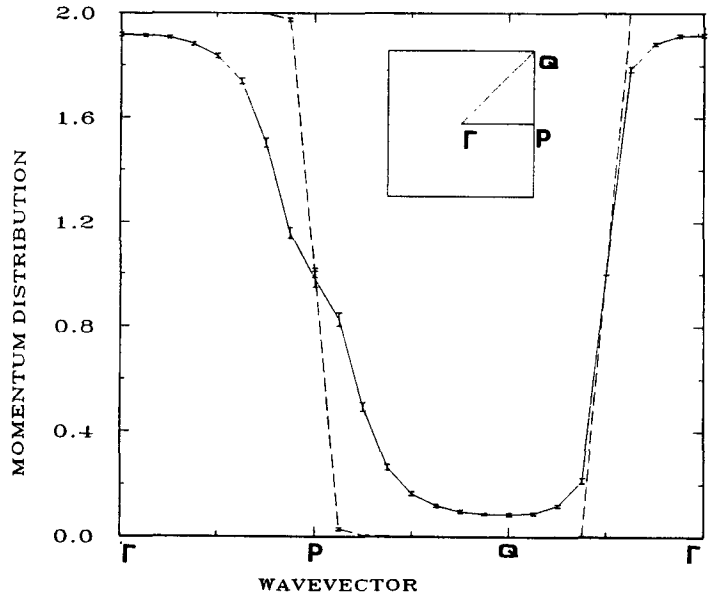

Figure 3. Momentum distribution of the half filled 2D 16×16 Hubbard model for U=0.5 (dashed line) and U=4 (continuous line). The imaginary time for this simulation was T=12. The ground state energy per site was $E_0 = -1.491$ for U=.5 and $-.85(7)$ for U=4. The corresponding HF values are -1.488 and $-.797$ The path in the Brillouin zone is shown in the inset. Note that the $Q\Gamma$ k-scale is compressed

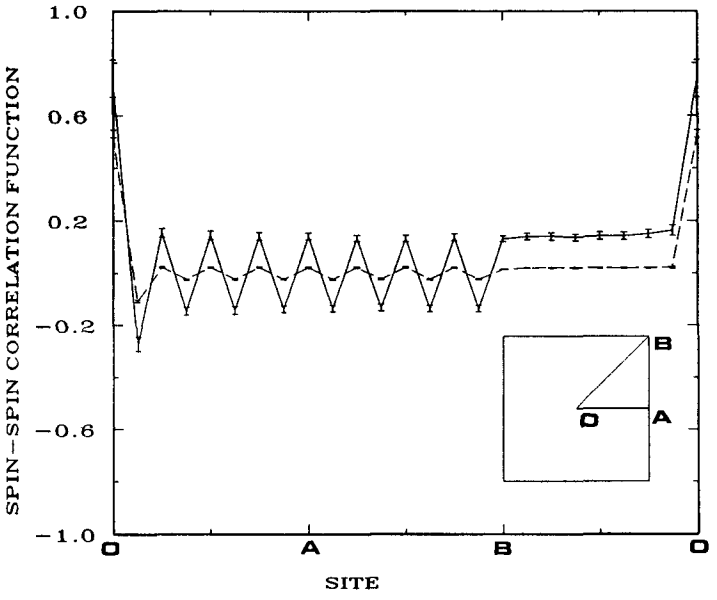

Figure 4. Spin-spin correlation function of a half-filled 2D 16×16 Hubbard model for U=0.5 (dashed line) and U=4 (continuous line). The path in the unit cell is shown in the inset.

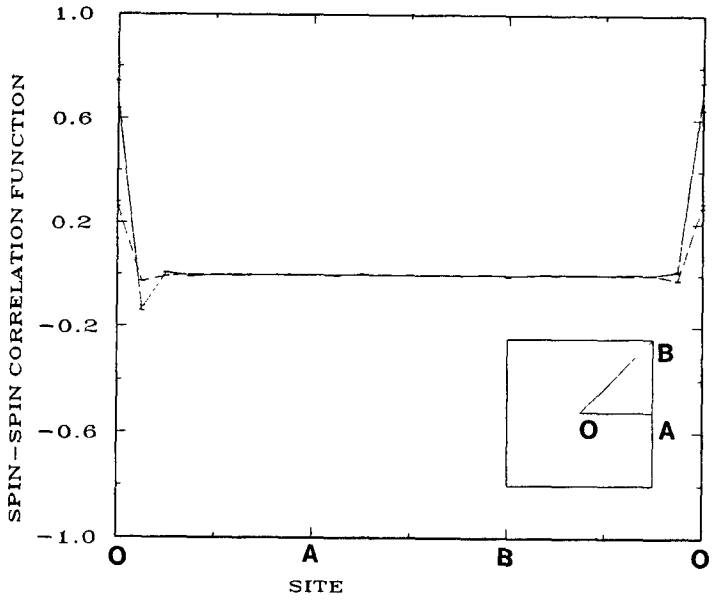

Figure 5. Spin-spin correlation function of a 2D 16×16 Hubbard model for U=4, $\nu=\frac{226}{256}$ (continuous line) and $\nu=\frac{74}{256}$ (dashed line). The path in the unit cell is shown in the inset.

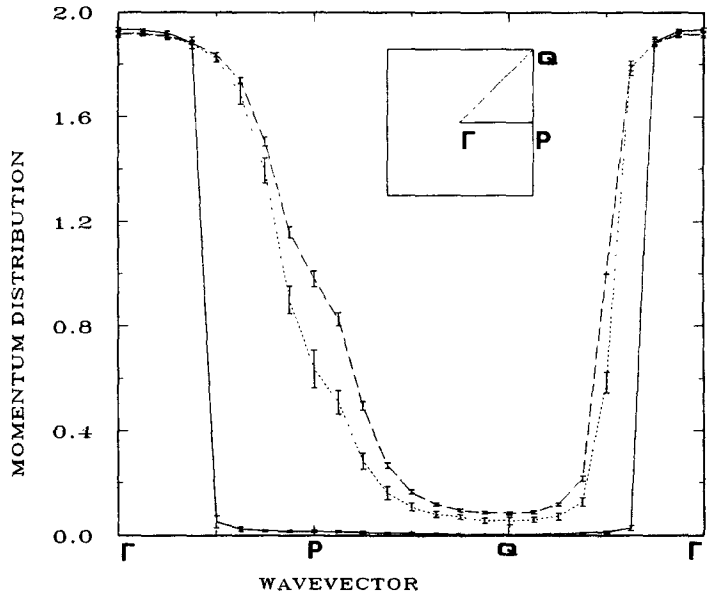

Figure 6. Momentum distribution of the 2D 16×16 Hubbard model with U=4,for $\nu=\frac{256}{256}$ (dashed line), $\nu=\frac{226}{256}$ (dotted line), and $\nu=\frac{74}{256}$ (continuous line). The path in the Brillouin zone is shown in the inset. The imaginary time was T=12 (half filled) and T=24 (less than half filled).

the momentum distribution $n(\mathbf{k})$ for the three values of δ considered above. Our

results, which are displayed in Fig. 6, show that the momentum distribution for the half-filled case is a smooth function consistent with the insulating character of the antiferromagnetic state. The momentum distribution of the half-filled AF Hartree-Fock state, shown by the dashed line of Fig. 7, is in fact rather similar to that of the true ground state of Fig. 6. The situation changes completely with moderate doping, $\delta = 12\%$. The new HF state displays a sharp dip corresponding to a Fermi surface (Fig.7). The true ground state $n(\mathbf{k})$ shown in Fig. 6, however, has no such dip, and roughly looks as though some kind of insulating character were preserved, in spite of the fact that magnetic order is destroyed. For heavy doping, finally ($\delta = 71\%$) a sharp Fermi surface is clearly recovered. We tentatively conclude that each of these three values of δ $(0, 12\%, 71\%)$ seems to correspond to a different phase, respectively an AF insulator, a yet unidentified non-magnetic non Fermi-liquid phase, and a Fermi liquid metallic phase. We do not know at present whether other phases might also appear. All in all, the 2D Hubbard model phase diagram appears richer than hitherto suspected.

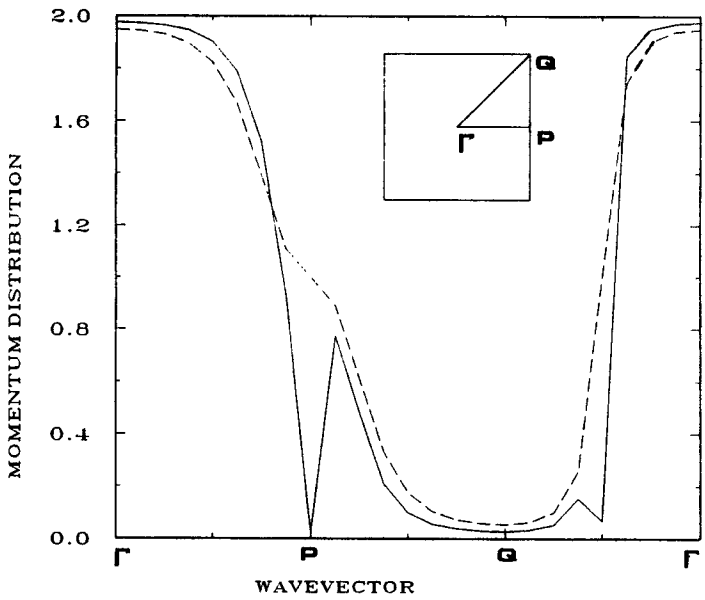

Figure 7. Momentum distribution of the Hartree-Fock AF solution of the 2D 16×16 Hubbard model with U=4. The dashed line correspond to half filling, whereas the continuous line corresponds to $\nu = \frac{220}{256}$.

In the 1D Hubbard model where only two different phases are expected from Lieb-Wu for $U > 0$, we have studied in detail the nature of the conducting case, which occurs for finite doping δ. Somewhat unexpectedly we find that a sharp jump in $n(\mathbf{k})$ occurs

at $k = k_F$ in all the cases considered, with no other significant features at $k = 2k_F$, or elsewhere. No sign of rounding of $n(\mathbf{k})$ was found on either sides of k_F. Fig. 8 shows the appearence of the jump in a 32-site calculation with only a minimal amount of doping ($\delta = 6\%$, or $\nu = \frac{30}{32}$).

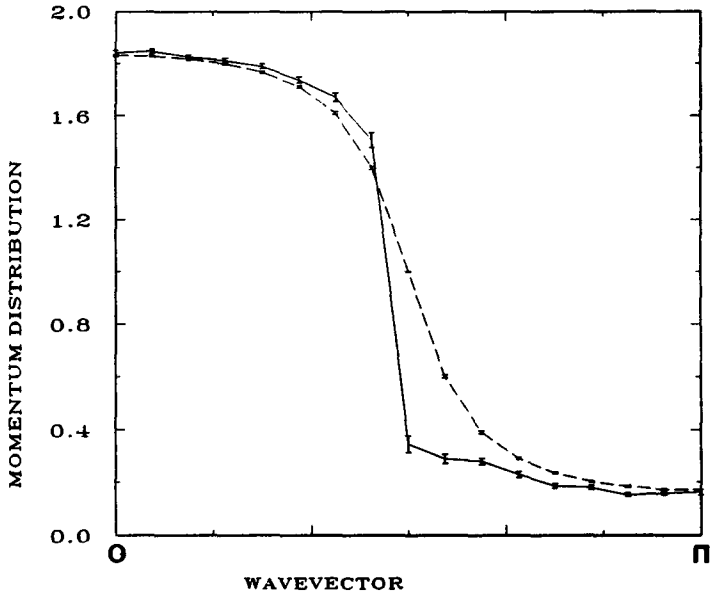

Figure 8. Momentum distribution of the 1D 32-sites Hubbard model with U=4. The dashed line corresponds to half-filling, whereas the continuous line corresponds to $\nu=\frac{30}{32}$. The imaginary time was T=12 in both cases. The kinetic energy per site calculated by means of the data shown in this Fig. are $E_{kin} = -.9728$ for the half filled case and $E_{kin}=-1.017$ for $\nu=\frac{30}{32}$. The corresponding exact values are $-.9757$ and -1.020 respectively. The calculated total energies are correspondingly $E_0=-.5726$ and $-.6576$, to be compared with the exact values $-.5743$ and $-.6567$. The exact values for $N_a=\infty$ at half filling is $-.5737$ [Z.G. Soos and S. Ramasesha, Phys. Rev. B 24,5410 (1984)]

The extreme sharpness of the jump is further confirmed by the larger size calculation which were extended till $N_a = 256$. Representative results for $\nu = \frac{102}{200}$ are shown in Fig. 9. At the Langevin level, we find that equilibration times at non zero doping are substantially shorter than for $\delta = 0$. The convergence in imaginary time is essentially the same. Fluctuations are still obviously present in this case, but, like all other cases studied, the jump of $n(\mathbf{k})$ occurs between the two k-values closest to k_F. We believe that this jump is a genuine feature of the finite size 1D Hubbard model. This is also confirmed by the excellent agreement with the corresponding finite size Lieb-Wu total and kinetic energy, the latter being very strictly connected with $n(\mathbf{k})$. Should this behaviour remain representative all the way to infinite size, this would imply a Fermi-

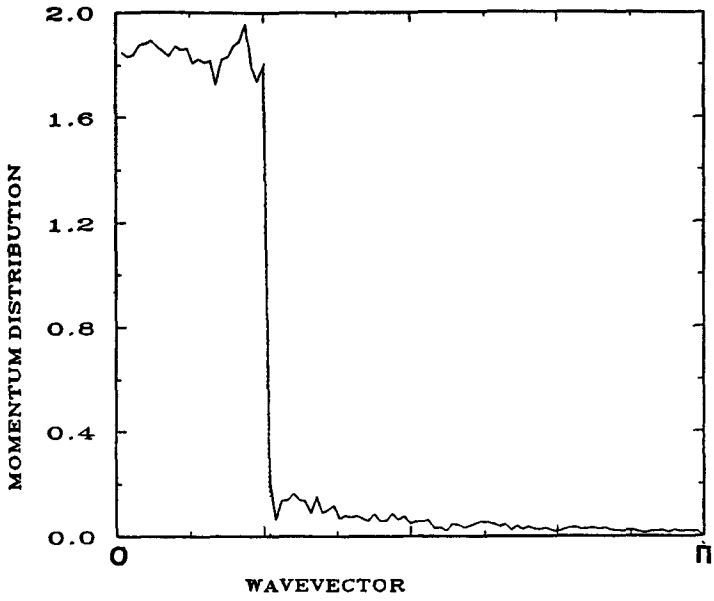

Figure 9. Momentum distribution of the 1D 200-site Hubbard model with U=4 for $\nu=\frac{102}{200}$ (continuous line). The imaginary time was T=16. The roughness of $n(\mathbf{k})$ is consequence of the statistical errors.

liquid behaviour of the doped 1D Hubbard model. Existing RG arguments, based on a mapping to the Tomonaga-Luttinger model (linearized dispersion), have suggested[2,10,11] the existence of a different state characterized by a power law singularity of $n(\mathbf{k})$ around k_F. Of course we cannot rule out either the existence of a power law singularity with an exceedingly small exponent, or a singular buildup of the singularity in the $N \to \infty$ limit. However we find no evidence of such singularity in the finite size systems, which behave as though they were arbitrarily close to Fermi-liquids.

Returning to the 2D Hubbard model, we are naturally led to speculate on the nature of the unidentified phase found for moderate doping. In this phase, holes do not appear to propagate as free entities, or else they would give rise to a Fermi jump. Various possibilities seem open, one of which might account for this behaviour. A hole could be bound either to another hole, or to a doubly occupied site. Alternatively, a hole could possibly "dissociate" into a holon-spinon pair, as advocated by the RVB model[4].

We are presently in the process of extending our studies to more appropriate correlation functions which should help to elucidate further these issues, as well as the possible existence of superconducting properties, or RVB fluctuations, in the 2D Hubbard model.

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