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LETTER TO THE EDITOR

Finite size scaling approach to the 1D Hubbard model

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Abstract. Finite size scaling is applied to the one-dimensional Hubbard model with the half filled energy band, at zero temperature. It is shown that, even for the scaling between small blocks of four, six and eight atoms, the essential singularity of the weak coupling limit is reproduced with remarkable accuracy, the error being less than 1% for the exponent and a few percent for the multiplicative constant. The results are discussed in comparison with the quantum renormalisation group approach, which fails to give the right exponent, and the advantages of the present method are pointed out.

In recent years, the Hubbard model has been the subject of numerous studies, both for its experimental implications (Jérome and Schulz 1982), and for its theoretical interest, leaving many open questions and being related to some other solid state and field theory models (Emery 1979). One of the important aspects of this model is its critical behaviour, on which we will concentrate in this letter.

The Hubbard model was defined (Hubbard 1963, 1964) to describe the correlations between electrons in narrow energy bands, including only the hopping of elcctrons between neighbouring atoms and the on-site interaction between them. Even such a simplified picture contains some essential features concerning the metal–insulator transition and the magnetic properties of physical systems.

The exact solutions are available for the one-dimensional case. Further investigations of the critical behaviour of the original model or its extended versions have been performed applying the approximate methods such as the parquet approximation (Bychkov *et al* 1966), bosonisation (Luther and Emery 1974), finite size extrapolations (Shiba and Pincus 1972), Monte Carlo simulations (Hirsch *et al* 1982) and different renormalisation group techniques (Chui and Bray 1978, Sólyom 1979, Emery 1979).

In particular, it was expected that the zero temperature critical behaviour of the (simple) Hubbard model would be successfully calculated by using the quantum real space renormalisation group (QRG) (Drell *et al* 1977, Jullien *et al* 1978) which was efficient in studying the ground state properties of a number of spin and fermion models. However, this approach, when tested on the soluble case (Hirsch 1980, Dasgupta and Pfeuty 1981), has encountered difficulties in the determination of the correct critical behaviour that could not be reduced by improving the approximation.

The aim of this letter is to propose finite size scaling as an alternative method which overcomes these difficulties and gives very accurate results in a technically simpler way.

We limit ourselves to the same, exactly solvable problem. We consider the one-dimensional Hubbard model with a half filled band at $T = 0$. The Hamiltonian is given

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by

$$H = t\sum_{i,\sigma}(c^{+}_{i,\sigma}c_{i+1,\sigma} + c^{+}_{i+1,\sigma}c_{i,\sigma}) + \tfrac{1}{2}U\sum_{i,\sigma} c^{+}_{i,\sigma}c_{i,\sigma}c^{+}_{i,-\sigma}c_{i,-\sigma} \tag{1}$$

where $c^{+}_{i,\sigma}$ and $c_{i,\sigma}$ are the creation and destruction operators for electrons with spin σ at atom i. As shown by Lieb and Wu (1968), in this case there is no metal–insulator transition at any finite $U>0$, the system being always insulating, but the energy gap vanishes when approaching $U=0$ with the essential singularity of the form $G = (8/\pi)\sqrt{U/t}\exp(-2\pi t/U)$. The ground state has an antiferromagnetic algebraic order. Both QRG calculations find the existence of the essential singularity, but with the exponent equal to 2 instead of 1.

Finite size scaling relies upon the ansatz (Fisher and Barber 1972) that, near the phase transition, any critical quantity C of the system which has finite size N in one direction and is infinite in the remaining directions satisfies the relation

$$C_N(U) = C_\infty(U)\cdot f(N/\xi_\infty), \tag{2}$$

where f is a homogeneous function and ξ is the correlation length for the infinite system. For quantum phase transitions at $T=0$, there is always one infinite 'direction' associated with the time, while the correlation length is expressed through the inverse energy gap between the ground state and the first excited state. U denotes the critical parameter. Equation (2) leads to a scaling relation of the same type as one obtained by the scale transformation in the infinite system

$$C_N(U) = (N/M)^{x/\nu}C_M((N/M)^{1/\nu}U). \tag{3}$$

x and ν are the critical exponents of C and ξ respectively, while C_N and C_M denote the critical quantity C for two different sizes. One way of extracting the critical behaviour is to linearise equation (3) around the fixed point as was done for a number of classical 2D and quantum 1D systems (for some references see Naghtingale 1982).

In the present problem, this procedure can be used to establish the exponential behaviour of the gap, but difficulties arise when one tries to extract the essential singularity critical exponent. Here, we adopt the procedure proposed by Roomany and Wyld (1980) which appeared to be more efficient, especially when dealing with the essential singularities. We thus consider the Callan–Symanzik β function $\beta = a\partial U/\partial a|_{\tilde{G}}$, where the constant of integration is the scaled gap; for size N it is equal to $\tilde{G}_N = N\cdot G_N$, since $G_N \sim 1/\xi_N$. a is the lattice constant, which can be expressed through N to obtain

$$\beta = -N\left.\frac{\partial U}{\partial N}\right|_{\tilde{G}_N} = \frac{2\ln(\tilde{G}_N/\tilde{G}_M)}{\ln(N/M)(G'_N/G_N + G'_M/G_M)}. \tag{4}$$

In the limit $N\to\infty$ this formula gives a more familiar expression $\beta = G_\infty/G'_\infty$, which relates β to the critical exponent σ. For the essential singularity of the form $G\sim\exp(-A/U^\sigma)$ it will be $\beta = U^{\sigma+1}/\sigma\cdot A$ (different from that in the case of a power law singularity $G\sim 1/U^x$, where $\beta = U/x$).

The results for $\tilde{G}_{N,M}$ were obtained by the exact numerical diagonalisation of the Hamiltonian (1) for the chains of four, six and eight atoms. The choice of the boundary conditions is important, since, for the finite system, the Fermi level oscillates as a function of N with periodicity 4. In such a case it is useful to take the modified boundary conditions (Spronken *et al* 1981) in order to be able to compare the results

for different sizes. Therefore, for four and eight atoms we have taken the periodic and for six atoms the anti-periodic boundary conditions. The calculations were performed in momentum space. Considerable reduction of the matrix sizes was achieved due to conservation of the total momentum k, the total magnetic momentum and the total number of electrons. Thus the results for four and six atoms were obtained by direct diagonalisation, while 618×618 matrices for the $N=8$ case were diagonalised using the Lanczos method.

It is particularly important to choose the correct energy levels related to the gap, since the difference between the two lowest levels does not necessarily correspond to it. For the chosen boundary conditions the lowest level is four-fold degenerate for $U=0$ and splits into four distinct levels for $U\neq0$. The analysis of the corresponding eigenvectors shows that, for small U, the first and fourth level belong to the same momentum subspace and are split by the Umklapp process. They should, therefore, correspond to the charge density wave gap and be related to the conductivity. The second and third level make part of the other momentum subspace and can be related to the spin density waves. Then, representing the gap as the difference between the fourth and first energy levels

$$\tilde{G}_N = N(E_4 - E_1) \tag{5}$$

we calculated the function β for different values of U in the interval between 0 and $0.01t$, where the factor $\sqrt{U/t}$ can be neglected. The parameter t has been taken equal to unity. The shape of β as a function of U corresponds to the exponential behaviour of $G(U)$, with the critical exponent σ and the multiplicative constant A presented in table 1. In comparison with the exact values, the results show very good accuracy, the exponent σ being determined with less than 1% error even for the scaling between chains of four and six atoms.

Table 1. Values of the essential singularity exponent σ and the multiplicative constant A for the scaling between different sizes M and N compared with the exact value for the infinite system.

M, N	σ	A
4, 6	0.992	6.250
6, 8	0.993	6.372
exact ($N=\infty$)	1	2π

In comparison with QRG one should note the following. Although apparently simple, the present problem is complex for the QRG, since it contains two types of degrees of freedom: charges and spins. They scale differently and both depend on U. Since the QRG keeps the Hamiltonian invariant, transforming the only parameter U, the resulting critical exponent contains the contributions from both degrees of freedom, which reduces the accuracy. Within renormalisation group methods, this inconvenience is avoided by introducing additional parameters into the Hamiltonian, which allows the separation of charge density waves from spin density waves (Emery 1979, Sólyom 1979). The advantage of the present method is that, within the one parameter Hamiltonian, it can treat the two degrees of freedom separately. This is made possible by choosing the levels corresponding only to the charge degrees of freedom and applying the scaling by keeping invariant the charge density wave gap.

In conclusion, by studying a one-dimensional example, we have shown that finite size scaling could be very efficient in studying the Hubbard model, both because of its accuracy and its ability, in comparison with QRG, to separate different degrees of freedom.

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