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The thermodynamical limit of strongly correlated systems obtained from small-size-cluster calculations

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Abstract. We study the properties of strongly correlated systems, calculating the self-energy of the electronic propagator of small-size clusters. We focus our attention on the one-dimensional Hubbard model. It is shown that for adequate sizes and boundary conditions, the self-energy of such a small cluster possesses the correct singular behaviour in the vicinity of the Fermi level for all values of the intra-atomic electron–electron interaction parameter U. The charge-transfer gap and other physical properties of the system are obtained at the thermodynamic limit. The survival of a single-pole singularity at $w = 0$ for the infinite-system self-energy constitutes a criterion for establishing whether the system is an insulator or a metal.

The properties of strongly correlated systems are attracting renewed interest in solid-state physics. Mainly due to the great complexity of the problem, it has not been possible to obtain exact solutions, except for very particular limits and systems. One of the simplest models which is supposed to possess the essential ingredients of highly correlated electrons is the Hubbard model. An exact analytical solution for the ground state of a one-dimensional (1D) system and its related properties was obtained many years ago [1–3]. A variety of approximate methods have been used, proving their capabilities as regards properly describing the known physics of the 1D system. They have also been used to study its other properties. These methods include diagrammatic summation [4], bosonization [5], renormalization group [6, 7] and conformal approaches [8, 9]. This has permitted a detailed knowledge of the problem to be obtained. It is now clear that in 1D the system is not a Fermi liquid, quasi-particles do not exist, there is no well defined Fermi surface and the occupation number is not discontinuous at the Fermi wavenumber. Although, at half-filling, the system is an insulator for any arbitrary small intra-atomic electronic repulsion parameter U, it is a metal for any other charge content. This unusual one-dimensional behaviour corresponds to what has been described as a Luttinger liquid. Although the above-mentioned techniques have given some important insights into the physics of higher-dimensional systems, the completeness of the knowledge that we possess for the 1D case is unfortunately lacking.

Alternative exact numerical solutions restricted to small clusters designed to represent 1D and 2D systems have been obtained [11]. Although good work has been carried out that is devoted to exact numerical calculation, this is a tool with severe shortcomings. Its capabilities

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are restricted to studying large energy excitations, local thermodynamic mean values and short-range correlations as functions of the parameters of the Hamiltonian. These limitations obviously derive from the finite size of the cluster studied. We know that this approach is in principle not appropriate for the 1D case for which the charge–charge and spin–spin correlations are long range in character, following asymptotic power laws with logarithmic corrections [10]. However, we were able to show that it is possible to obtain some insight into the 1D physics of an infinite system from the results obtained by exact diagonalization of a finite cluster. This lends support to our claim of its applicability for studying 2D and 3D systems where physical quantities have a more local character. In order to do this, it is necessary to know what the properties are and under what conditions the exact solution for a small-size system contains information which is relevant in the thermodynamic limit. It is clear that the physics of a finite cluster introduces an energy scale which follows from the energy discretization of the one-particle spectrum and that depends upon the size of it. The cluster has to be designed in such a way that this spurious energy scale, which does not exist in the thermodynamic limit, is not present for the charge excitations, at least in the vicinity of the Fermi energy. The electron–hole symmetry (EHS) at half-filling is another property which has to be preserved in the cluster, as it is an essential property of the infinite system.

In this paper we study the electronic propagator of a small 1D cluster and show how some of the properties of an infinite Hubbard chain can be deduced from it. We show that the propagator self-energy in the vicinity of the Fermi level and clusters and boundary conditions correctly chosen guarantee a good physical description in the thermodynamic limit.

We use the EHS property to derive an important analytical behaviour of the propagator self-energy.

In general, the one-particle propagator (OPP) can be expressed as

$$G_k(w) = \sum_m \frac{|\langle m|C_{k,\sigma}|0\rangle|^2}{w + \delta E_{m,k}^{N-1} - \mathrm{i}\eta} + \sum_n \frac{|\langle n|C_{k,\sigma}^\dagger|0\rangle|^2}{w - \delta E_{n,k}^{N+1} + \mathrm{i}\eta}. \tag{1}$$

The frequency w is measured from the chemical potential of the system. $\delta E_{m,k}^{N-1}$, $\delta E_{n,k}^{N+1}$ are the energies of the excitations $|m\rangle$, $|n\rangle$ of $N-1$ and $N+1$ particles respectively and $|0\rangle$ is the N-particle ground state. At $U = 0$ these energies are equal to the absolute value of the free-electron energy $|e_k|$. We define the quasiparticle weights as

$$a_{k,m} = |\langle m|C_{k,\sigma}|0\rangle|^2 \tag{2}$$

$$b_{k,m} = |\langle n|C_{k,\sigma}^\dagger|0\rangle|^2. \tag{3}$$

The ground state of the system has total momentum $K = 0$. We analyse the OPP for the Fermi wave vector $k_f = \pi/2$. Due to the EHS, at half-filling we can write that

$$a_{k_f,n} = b_{k_f,m} = a_m$$
$$\delta E_{m,k_f}^{N+1} = \delta E_{m,k_f}^{N-1} = \delta E_m. \tag{4}$$

The expression (1) for the OPP can be written as

$$G_{k_f}(w) = \sum_m \frac{2a_m w}{w^2 - \delta E_m^2} + \mathrm{i}g_{k_f}(w) \tag{5}$$

where

$$g_k(w) = \sum_m \mathrm{i}\pi(\delta(w + \delta E_{m,k}) - \delta(w - \delta E_{m,k})). \tag{6}$$

Defining the self-energy $\Sigma_k(w)$ from the equation

$$G_k(w) = (w - \Sigma_k(w))^{-1} \tag{7}$$

and using equation (4) at $k = k_f$, it turns out that

$$\Sigma_{k_f}(w) = w - \left[w \sum_m \left(\frac{2a_m}{w^2 - \delta E_m^2} \right) + \mathrm{i} g_{k_f}(w) \right]^{-1}. \tag{8}$$

Now, let us suppose that there is a gap in the excitation spectrum of the problem. In this case, in the limit $w \to 0$, the self-energy is real and we can write (8) as

$$\Sigma_{k_f}(w) = \frac{c}{w} + w(1-b) \tag{9}$$

where

$$c = \left(\sum_m \frac{2a_m}{\delta E_m^2} \right)^{-1} \tag{10}$$

$$b = -\sum_m \frac{4a_m}{\delta E_m^2} \left(\sum_m \frac{2a_m}{\delta E_m^2} \right)^{-2}. \tag{11}$$

Equations (9), (10) show that the existence of a gap gives rise to a self-energy with a single pole at the Fermi level. Note that this is true even when in the thermodynamic limit the OPP in general has no single poles and instead has a branch cut along the frequency axis [12]. This is a property which follows exclusively from the EHS and it is valid in any dimension when the system has a gap at the Fermi level. Then, from (7), it is easy to show that the gap Δ is given by

$$\Delta = 2\sqrt{c/(1-b)}. \tag{12}$$

The analysis for $k \neq \pi/2$ is similar, but in this case $a_{k,m} \neq b_{k,m}$. Then we obtain for the OPP the following expression:

$$G_k(w) = \sum_m (a_{k,m} + b_{k,m}) \frac{w + [(b_{k,m} - a_{k,m})/(b_{k,m} + a_{k,m})]\delta E_{m,k}}{w^2 - \delta E_{m,k}^2} + \mathrm{i} g_k(w). \tag{13}$$

At $w = 0$ the OPP and the self-energy are analytical functions. For the rest of the spectrum outside the gap, the OPP has a branch cut which coincides with the support of the density of states of the system.

For a finite-size system the branch cut transforms into single-pole singularities located at the excitation energies, which are related to the single-pole singularities of the self-energy. In fact, the self-energy can be written as

$$\Sigma_k(w) = w - \left(\prod_m (w^2 - \delta E_{m,k}^2) \right) \Big/ P_{k,2M-1}(w) \tag{14}$$

$$P_{k,2M-1}(w) = \sum_m (a_{k,m} + b_{k,m}) \left(w + \frac{b_{k,m} - a_{k,m}}{b_{k,m} + a_{k,m}} \delta E_{l,k} \right) \prod_{l \neq m} (w^2 - \delta E_{l,k}^2) \tag{15}$$

where M is the number of excitations of total momentum $K = k$ and $P_{k,2M-1}(w)$ is a polynomial of degree $2M-1$. The roots of this polynomial are the single poles of the self-energy, each one intercalated in $(\delta E_{m,k}, \delta E_{m+1,k})$. It is evident from (14) that in the case where $k = \pi/2$, i.e. when $b_{k,m} = a_{k,m}$, the self-energy has a single pole at $w = 0$. It is important to call attention to the behaviour of these poles in the thermodynamic limit. The residues of the OPP poles tend to a finite value in the vicinity of the Fermi level where the system is a Fermi liquid and there are quasi-particle excitations. This gives rise to a discontinuity in the occupation number $n_k = \langle C_k^\dagger C_k \rangle$ at $k = k_f$. However, when the system is a Luttinger liquid, the weights of the poles tend to zero for an infinite system. This reflects the absence of

well defined one-particle excitations near the Fermi energy. The self-energy has very similar analytical properties. However, even for the case of a Luttinger liquid, in the presence of a gap at the Fermi level, the residue of the $w = 0$ pole tends to a finite value. The analytical structure of the self-energy corresponds in this case to a single isolated pole at $w = 0$ and a branch cut in the spectrum region outside the gap. In contrast, when no gap is present in the spectrum, the excitation energies can be zero and in this case the branch cut includes the origin. The self-energy of a finite-size cluster will always have a $w = 0$ pole. However, it is not maintained as a single-pole singularity because its residue tends to zero in the thermodynamic limit.

The difference between the two cases can easily be detected by analysing the singularity at $w = 0$, increasing the size of the system and extrapolating the result to infinite length.

We have applied these ideas to a 1D Hubbard model defined on a cluster of L sites given by the Hamiltonian

$$H = \sum_{l=1}^{L} C^{\dagger}_{l+1,\sigma} C_{l,\sigma} + \text{h.c.} + U \sum_{l=1}^{L} n_{l,\uparrow} n_{l,\downarrow} \tag{16}$$

where the notation is as usual. The problem can be defined with open (OBC) or closed boundary conditions. In this latter case they can be periodic (PBC) or anti-periodic (APBC).

We choose a size and a boundary condition which incorporate the relevant properties of the thermodynamic limit [13]. They are twofold: the EHS which is reflected in the self-energy at $k = k_f = \pi/2$ and the existence of excitations of zero energy for the non-interacting system. The main issue here is that the energy difference between the kinetic energy levels is $\sim t/L$. This gives rise, in the non-interacting infinite system ($L \to \infty$), to a continuous spectrum of excitations. The kinetic energy levels will be strongly perturbed by the interaction when the cluster size L satisfies $L \gg t/U$. For moderate values of the parameter U, this limit is numerically not feasible because it corresponds to a very large system.

For the small-size clusters accessible to numerical study, the discrete character of the spectrum introduces a new energy scale, t/L. The influence of this property of the cluster, absent in the infinite system, has to be adequately treated in order to allow us to extract the correct physics of the thermodynamic limit.

Two qualitatively different situations appear according to whether the kinetic spectrum for the one-particle system is degenerate at the Fermi level or not. In the non-degenerate case there is a gap at the Fermi level in the non-interacting excitation spectrum of the order of t/L. This is the case of a cluster with PBC and $L = 2(2n+1)$ or APBC and $L = 4n$, with n an integer. This gap inhibits the effect of the correlation. It is obvious that this cluster violates the EHS, which, according to the discussion above, controls the analytical properties of the self-energy at the Fermi level. The response of the system to U in this case is perturbative. Near the Fermi level, all of the diagonal and non-diagonal components of the self-energy are completely regular and the effect of the interaction appears essentially as a displacement $U/2$ of the diagonal self-energy. Taking the system to the thermodynamic limit, these self-energies will reproduce a homogeneous restricted Hartree–Fock solution to our problem. This approximation is not capable of producing an insulating gap, which is known to be an essential property of 1D highly correlated electrons. These systems are Mott insulators for any arbitrary value of the parameter U. This property will never be obtained from clusters with these sizes and boundary conditions.

The degenerate case is a different physical situation, since the non-interacting electronic excitations have no gap at the Fermi level and the EHS is preserved. We can obtain this case by choosing sizes or boundary conditions as follows: PBC and $L = 4n$ or APBC and $L = 2(2n + 1)$. In these cases, as the Fermi level is degenerate, the response of the system to U is highly non-perturbative, even for $U \ll t/L$. To incorporate an extra particle into

the finite system requires in this case an extra energy proportional to U. The single-pole singularity at $w = 0$ controlling the gap is now present in the self-energy, as is shown in figure 1. Decomposing (14) into simple fractions, the self-energy can be written as

$$\Sigma_k(w) = \sum_m \frac{a_{k,m}}{w - w_{k,m}} + \frac{U}{2} + 2\cos(k) + f(w) \tag{17}$$

where the $w_{k,m}$ correspond to the roots of the polynomial $P_{k,2M-1}(w)$ given in (15) and $f(w)$ is an analytic function. The residues $a_{k,m}$ and the poles $w_{k,m}$ have been determined by diagonalizing finite-size clusters of length $L = 2, 4, 6, 8, 10$, with adequate boundary conditions, as already discussed. Using a Lanczos algorithm we obtain the ground state and the Green

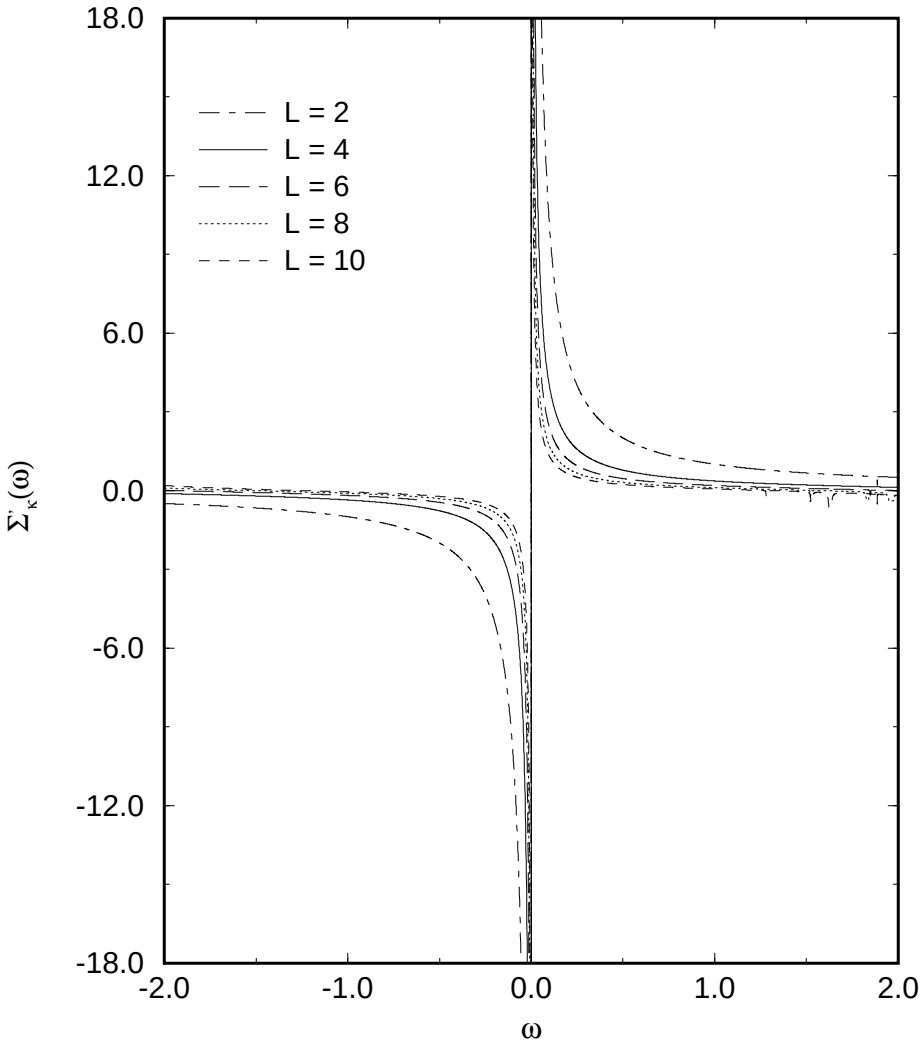

Figure 1. $\Sigma'_{\pi/2}(w) = \Sigma_{\pi/2}(w) - U/2$ for $U = 2$. The coefficients c are 1, 0.3956, 0.2386, 0.1691, 0.1306 for $L = 2, 4, 6, 8, 10$ respectively. The extrapolated value is 0.0069. The coefficients b are 0, -0.0319, -0.0468, -0.0583, -0.0685 in the same order as before. The extrapolated value is -0.1555.

functions of the clusters [11]. From the knowledge of the Green function we get diagonal and non-diagonal components of the self-energy $\Sigma_l(w)$ compatible with the size of the cluster considered. We perform the Fourier transformation and obtain the residues $a_{k,m}$ as functions of the length of the cluster and U. In the thermodynamic limit only the residue of the pole at $w = 0$ for $k = \pi/2$ survives, as discussed above, indicating the existence of a gap. The other excitations are distributed densely along the real axis with a residue going to zero, indicating the existence of a branch cut and characterizing the system as a Luttinger liquid.

In order to illustrate this behaviour, we represent in figure 2 the weights of the $w = 0$ singularity for $k = \pi/2$ and of the singularity corresponding to the excitation of least energy for $k = 0$. It is clear from the figure that while the $w = 0$ pole has a residue that tends to a finite value in the thermodynamic limit, the other goes to zero exponentially as the size is increased. It is this rapid convergence to the extrapolated values that gives rise to a very sensitive diagnostic as regards whether a single $w = 0$ pole in the thermodynamic limit exists or not, and, as a consequence, as regards the existence of a gap.

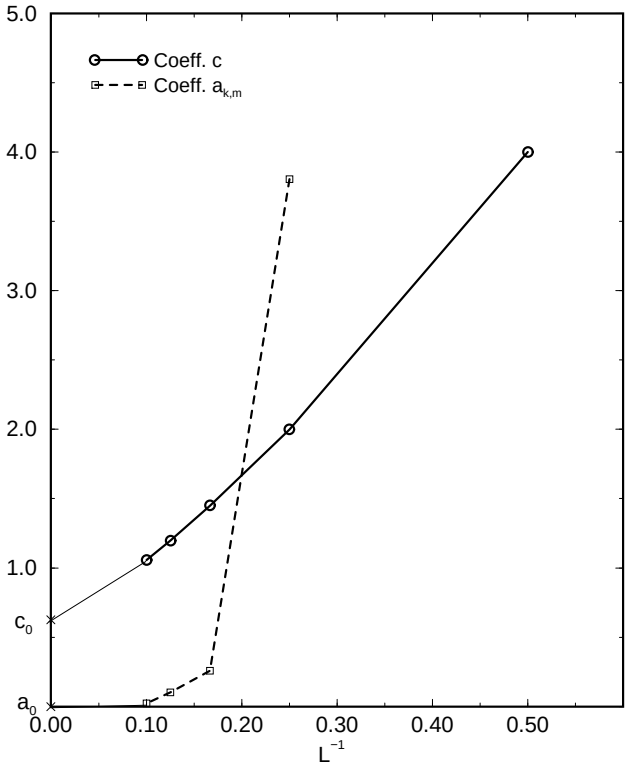

Figure 2. Coefficients of the self-energy singularities for $k = \pi/2$ and $k = 0$ with $U = 4$. The extrapolated value for $k = \pi/2$ is $c_0 = 0.6266$. For $k = 0$ and $m = 0$ the extrapolated value is $a_0 = 0$.

From the extrapolated weight of the singularity at $k = \pi/2$ we can obtain the gap, using equation (12). In figure 3 we compare it with the analytical result for several values of U. We get, for moderate values of U, an exact result for the insulating gap. For larger values, $U \geqslant 8$, an accurate value for the gap requires the calculation of extra terms in (9) ($\sim w^2$, w^3, ...).

Summarizing, in the thermodynamic limit, the self-energy of a system with EHS and a

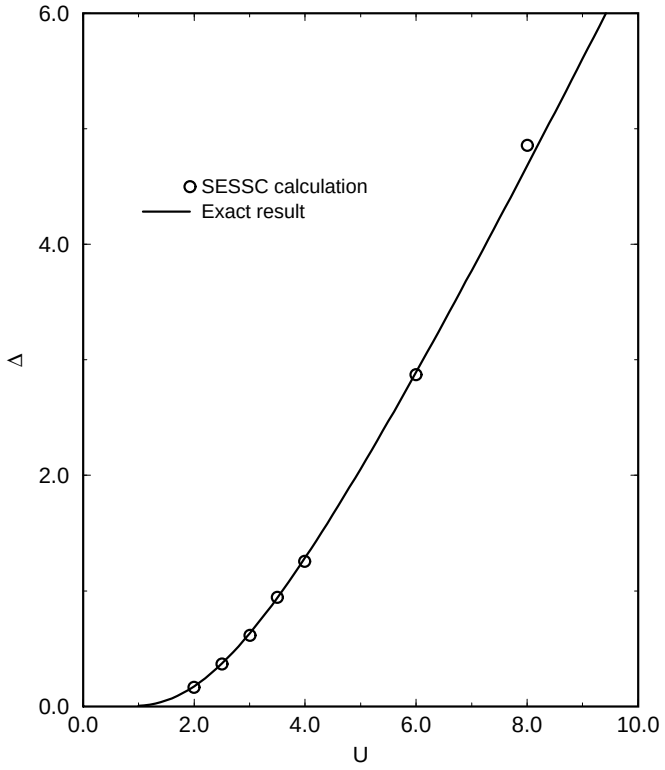

Figure 3. The gap versus U; the self-energy small-size-cluster (SESSC) calculation and the analytical result.

gap has a single-pole singularity at $w = 0$. We were able to show that, by choosing appropriate sizes and boundary conditions, this property of the system can be extracted from the singular behaviour of the small-cluster self-energy $\Sigma_k(w)$. This singularity exists for any value of U and has the correct trend as the size of the cluster is increased. This study suggests the existence of an insulating gap when the residues of the self-energy single-pole singularity at the Fermi level are finite at the thermodynamic limit. In this direction, investigations of clusters capable of representing a 2D system are in progress.

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