Susceptibility of the one-dimensional, dimerized Hubbard model

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Abstract

We show that the zero temperature susceptibility of the one-dimensional, dimerized Hubbard model at quarter-filling can be accurately determined on the basis of exact diagonalization of small clusters. The best procedure is to perform a finite-size scaling of the spin velocity $u_\sigma$, and to calculate the susceptibility from the Luttinger liquid relation $\chi = 2/\pi u_\sigma$. We show that these results are reliable by comparing them with the analytical results that can be obtained in the weak and strong coupling limits. We have also used quantum Monte Carlo simulations to calculate the temperature dependence of the susceptibility for parameters that should be relevant to the Bechgaard salts. This shows that, used together, these numerical techniques are able to give precise estimates of the low temperature susceptibility of realistic one-dimensional models of correlated electrons.

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The properties of correlated electrons are fairly well understood in one dimension [1,2]. The low-energy physics of systems with low lying charge and spin excitations is well described by the Tomonaga-Luttinger fixed-point, while the properties of systems with a gap in the charge or in the spin sector can be inferred from those of the half-filled Hubbard model or of the Luther-Emery model respectively. When it comes to a precise understanding of the one-dimensional properties of real materials, like the organic conductors, this is not sufficient however. The ultimate goal is to understand both the high and low energy properties of a given material in terms of a few parameters describing the basic electronic processes, namely hopping integrals and Coulomb repulsions. For instance, for the Bechgaard salts, a good candidate to describe the electronic properties is given by the quarter-filled, dimerized Hubbard model [3] defined by the Hamiltonian

$$H = -t_1 \sum_{i \text{even}, \sigma} (c_{i,\sigma}^\dagger c_{i+1,\sigma} + \text{h.c.}) - t_2 \sum_{i \text{odd}, \sigma} (c_{i,\sigma}^\dagger c_{i+1,\sigma} + \text{h.c.}) + U \sum_i n_{i\uparrow} n_{i\downarrow}$$  \hspace{1cm} (1)

The parameters of this model are: i) a hopping integral $t_1$ for the short bonds; ii) a hopping integral $t_2$ ($\leq t_1$) for the long bonds; iii) an on-site repulsion $U$. In the following, energies will be measured in units of $t_1$, and the basic dimensionless parameters are $t_2/t_1$ for the dimerization and $U/t_1$ for the Coulomb interaction. To check whether this is a fair description of the low energy properties, one needs reliable estimates of the quantities that are accessible experimentally. For instance, the activated behaviour of the resistivity at low temperature in (TMTTF)$_2$PF$_6$ is believed to be due to a small gap in the charge spectrum [4]. To get a quantitative estimate of the charge gap in the model of Eq. (1) is a difficult – but not hopeless – problem that we have addressed in a previous paper [5]. Another useful probe of the low energy physics is provided by the static susceptibility, which has been measured quite extensively as a function of temperature for the Bechgaard salts [4]. The interpretation that has been proposed so far is based on analytical results obtained in the weak-coupling limit of the non-dimerized model. This is probably a good approximation for (TMTSF)$_2$PF$_6$ because the dimerization is small, but not for (TMTTF)$_2$PF$_6$, in which case the ratio $t_2/t_1$ is about 0.7, and a calculation that takes the dimerization into account
should be done before a reliable interpretation of the data can be tried. Dimerization is actually a very common phenomenon in one-dimensional conductors, and such a calculation is likely to be useful in other contexts as well.

Surprisingly enough, it seems that there has not been any serious attempt at calculating the susceptibility of a dimerized model. Even for the Hubbard model, to which most of the effort has been devoted because it is soluble with the Bethe ansatz \cite{6}, the information that can be found in the litterature is not complete. The susceptibility has been calculated at zero temperature for any density by Shiba \cite{7} with the Bethe ansatz equations, but its temperature dependence could be determined along these lines only at half-filling \cite{8}. As a consequence, Torrance et al \cite{9} had to use approximate results obtained in the limiting cases of weak and strong on-site repulsion to analyze the susceptibility of TTF-TCNQ because the band-filling is not 1 but 0.59. A few years later, the temperature dependence of the susceptibility for the quarter-filled case and for $U/t = 4$ was determined through Monte Carlo simulations by Hirsch and Scalapino \cite{10}, but this was just intended as an illustration, and the precision was not good enough at low temperature for these results to be used in the interpretation of experimental results. In fact, the only attempt at calculating the temperature dependence of the susceptibility away from half-filling is due to Bourbonnais \cite{11}. His calculation is based on g-ology. The fact that the system is not half-filled is taken into account by neglecting the umklapp term. While this calculation seems reliable for not too large values of $U/t$ and at low temperatures, it clearly fails at higher temperature, the susceptibility diverging instead of vanishing as $1/T$.

In the present paper, we show that it is now possible to get accurate results for both the zero-temperature value and the temperature dependence of the susceptibility for one-dimensional models that do not have an exact solution by using standard numerical techniques together with analytical results in various limits. We have decided to concentrate on the model of Eq. (1) because it has a direct relevance to the Bechgaard salts, for which extensive experimental data are available, but the same approach can in principle be used for any model, with hopefully the same success.
Numerically, there are a priori several ways to calculate the susceptibility. One possibility is to go back to the original definition of the susceptibility as the derivative of the energy with respect to the magnetization evaluated for vanishing magnetization. This is not so accurate however because, with finite clusters, one has only values of the energy for discrete values of the total magnetization, and one first has to do a linear fit of the energy as a function of magnetization for small values of the magnetization. This procedure turns out to be rather arbitrary for the model of Eq. (1) when the repulsion is large. For one-dimensional systems, there is another way to calculate the susceptibility. Unless there is gap in the spin sector, the low energy spin excitations of electrons interacting through repulsive interactions can be described by a Luttinger liquid with a velocity $u_\sigma$, and the susceptibility can be obtained as $\chi = 2/\pi u_\sigma$. One route to the susceptibility is then to determine $u_\sigma$ numerically from exact diagonalization for small clusters. There are again several possibilities to extract this velocity. When $t_2/t_1 \neq 1$, we have shown that there is a gap in the charge sector of the model of Eq. (1). The ground-state energy is then expected to scale with the number of sites $L$ as

$$E_0 = \epsilon - \frac{\pi u_\sigma c}{6L^2} + o\left(\frac{1}{L^2}\right)$$

where $\epsilon$ is the energy density in the thermodynamic limit, and where the central charge $c$ should be equal to 1. In the present case, this cannot be a good way to determine $u_\sigma$. First, there are logarithmic corrections to the coefficient of the $1/L^2$ term which makes the estimate based on small clusters not very accurate. Second, and more importantly, this scaling behaviour is probably not satisfied for the sizes we can study with exact diagonalization. The reason is quite simple: When the dimerization is very small, the gap $\Delta_c$ in the charge sector is also very small. Now, the scaling of Eq. (2) can be observed only when the size of the systems is larger than the correlation length associated with this gap, which is given by $\xi \sim u_c/\Delta_c$, where $u_c$ is the slope of the dispersion of the charge excitations for energies larger than the gap. If the systems are small, the scaling of the ground-state will probably be closer to the formula for systems without a gap in the charge sector, which is similar to
Eq. (2), but with $u_\sigma$ replaced by $u_\sigma + u_c$, and Eq. (2) would provide a totally unreliable estimate of $u_\sigma$.

So it seems that the best way to determine $u_\sigma$ is to look at the spectrum directly, and to determine the slope of the spin excitations. More precisely, the finite-size estimate of $u_\sigma$ is given by

$$u_\sigma(L) = \frac{E(k_0 + 2\pi/L; S = 1; L) - E(k_0; S = 0; L)}{2\pi/L}$$

(3)

where $k_0$ is the momentum of the ground-state, and where $E(k; S; L)$ is the lowest energy in the subspace of states of momentum $k$ and total spin $S$ for a system of size $L$. This quantity is expected to go to the value $u_\sigma$ of the infinite system with dominant corrections of order $1/L$. We have calculated $u_\sigma(L)$ for systems with 8, 12 and 16 sites, and for several values of $t_2/t_1$ and $U/t_1$. This scaling was in most cases already very accurately satisfied. Small but not negligible deviations occurred for large values of $U/t_1$. As the form of the next-to-leading order corrections is not clear, we have used the systems with 12 and 16 sites to perform the $1/L$ extrapolation. The results for $\chi$ are given in Fig. 1.

We have performed several checks to convince ourselves that these estimates of the zero-temperature susceptibility were accurate. First, when $t_2/t_1 = 1$, the model of Eq. (1) is nothing but the Hubbard model. Solving numerically the equations of the Bethe ansatz, Shiba [7] calculated the susceptibility for several values of the density and of $U$. Our results are in perfect agreement with the results he quoted for quarter-filling.

In the weak-coupling limit, one can use $g$-ology to determine the corrections to the spin velocity. This leads to the following expression for the susceptibility:

$$\chi = \frac{2}{\pi v_F} \left(1 + \frac{U}{2\pi v_F}\right)$$

(4)

and $v_F = 2t_1t_2/\sqrt{t_1^2 + t_2^2}$ for the model of Eq. (1). This is again in very good agreement with the slopes we have obtained numerically for small values of $U/t_1$.

Given the uncertainty of our numerical procedure for large values of $U/t_1$, it is also very important to check the results that we have obtained in that limit. This turns out to be
possible along the lines we used to calculate the $1/U$ corrections to the charge gap [5]. When $U/t_1$ is very large, the ground-state is approximately given by the product of the spinless fermion Fermi sea with the ground-state wave function of the spin-1/2 Heisenberg model, the number of spins being equal to the number of electrons in the original model [14]. The coupling between the spins is described by an effective exchange integral $J_{\text{eff}}$ given by

$$J_{\text{eff}} = \frac{t_1^2 + t_2^2}{2U} - \frac{2(t_1^2 - t_2^2)}{\pi^2 U} K^2 \left( \frac{2\sqrt{t_1 t_2}}{t_1 + t_2} \right).$$

(5)

where

$$K(q) = \int_0^{\pi/2} \frac{d\phi}{\sqrt{1 - q^2 \sin \phi^2}}$$

(6)

is an elliptic integral of the first kind. The susceptibility is given in terms of $J_{\text{eff}}$ by [14]

$$\chi = \frac{1}{\pi^2 J_{\text{eff}}}.$$  

(7)

This result can be seen as a generalization of the result obtained by Klein and Seitz [15] for the Hubbard model. To compare with our results, we have plotted $\chi/U$ as a function of $1/U$, the result for $1/U = 0$ being deduced from the previous equations. The agreement is satisfactory. For large $U$, our numerical results for $\chi/U$ are slightly scattered, but they are consistent with the infinite $U$ result. We consider this agreement as a strong support in favour of this procedure to estimate the zero temperature susceptibility of one-dimensional models of correlated electrons for large values of the repulsion.

Quite independently from these results, information on the susceptibility at moderate to high temperatures can be obtained from Monte Carlo simulations. Experimentally, the temperature dependence of the susceptibility is usually known quite accurately, and its interpretation is not ambiguous in the sense that it gives access to the ratio $U/t$, which is a measure of the size of correlations, even if one does not know the value of the hopping integrals accurately. This should be contrasted to the low temperature value of the susceptibility: To give information on the size of correlation, this quantity has to be compared with estimates for non interacting electrons, and, for molecular conductors, these estimates are not reliable if they are deduced solely from band structure calculations.
The world-line algorithm of Hirsch et al [16] is known to be very convenient for one-dimensional models, and we have used it to determine the temperature dependence of the susceptibility for two sets of parameters: \( U/t_1 = 4, t_2/t_1 = 1 \), which should be reasonable for (TMTSF)_2PF_6, and \( U/t_1 = 8, t_2/t_1 = .7 \), which should be reasonable for (TMTTF)_2PF_6. In their original study of the extended Hubbard model, Hirsch et al worked at temperatures such that the finite size effects were smaller than the statistical errors. In our case, we need to go to temperatures that are small enough to make the link with the zero temperature results obtained with exact diagonalization. So we had to obtain results with statistical errors small enough to allow meaningful extrapolations. More precisely, we had to do three extrapolations. First, in the algorithm we have used, the magnetization is a conserved quantity. So, to get the static susceptibility, one has to extrapolate the finite \( q \) results to get the zero-\( q \) value of the susceptibility. Practically, this is done by fitting the results at small \( q \) with a parabola. Then, there is the systematic error due to the Trotter decomposition which goes as \( \Delta \tau^2 \), and which we eliminated by fitting the results obtained for different numbers of temperature slices. Finally, for the lowest temperatures studied, the finite-size effects were not negligible, and, by analogy with the procedure used for the zero-temperature susceptibility, we performed a linear fit in \( 1/L \) of the results obtained for different sizes to go to the thermodynamic limit. The error bar depicted on the figure is the largest of the statistical errors obtained for the various sizes and time-slice numbers for a given value of the temperature. The results are shown in Fig. 3. The agreement with the zero-temperature result is very good. This is particularly satisfactory for the case \( U/t_1 = 8, t_2/t_1 = .7 \), because this was already in the region where the finite-size corrections to \( u_\sigma \) were not purely \( 1/L \) for the small systems we could study with exact diagonalization.

As far as the Bechgaard salts are concerned, we will limit ourselves to a few remarks. A more complete account of these results, together with the interpretation of several other experimental data, will be given elsewhere. Let us note for the moment that the present results roughly confirm the interpretation given by Wzietek et al [4] for (TMTSF)_2PF_6: Our result for the temperature dependence of the susceptibility for \( U/t_1 = 4, t_2/t_1 = 1 \) is
consistent with the results of Bourbonnais. For \((\text{TMTTF})_2\text{PF}_6\), our results suggest that the
dimerization reduces the temperature dependence of the susceptibility, so that the analysis
of Wzietek et al, which did not take the dimerization into account, leads to an underestimate
of \(U/v_F\) in that compound.

In conclusion, we have shown that it is possible to obtain accurate results concerning
the susceptibility of one-dimensional models of correlated electrons that cannot be solved
exactly by Bethe ansatz by using numerical techniques and approximate methods in various
limits. A finite-size scaling of the spin velocity deduced from the spectrum obtained by exact
diagonalization provides good values of the zero-temperature susceptibility, while standard
Monte Carlo simulations give information on the temperature dependence that seems accu-
rate enough to allow an interpretation of the experimental data obtained on the Bechgaard
salts. It is our hope that this work will encourage experimentalists to try to interprete the
low energy results they can obtain for one-dimensional conductors in terms of microscopic
models.

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FIGURES

FIG. 1. Zero temperature susceptibility as a function of $U/t_1$ for several values of the dimerization: a) $t_2/t_1 = 0.4, 0.5, ..., 1$ from top to bottom; b) $t_2/t_1 = 0.1, 0.2, 0.3$ from top to bottom.

FIG. 2. $\chi t_1/U$ as a function of $t_1/U$ for several values of the dimerization: a) $t_2/t_1 = 0.4, 0.5, ..., 1$ from top to bottom; b) $t_2/t_1 = 0.1, 0.2, 0.3$ from top to bottom.

FIG. 3. Temperature dependence of the susceptibility for: a) $U/t_1 = 4$, $t_2/t_1 = 1$; b) $U/t_1 = 8$, $t_2/t_1 = 0.7$. 

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