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2008 J. Phys.: Condens. Matter 20 304212

(http://iopscience.iop.org/0953-8984/20/30/304212)

IOP PUBLISHING JOURNAL OF PHYSICS: CONDENSED MATTER

J. Phys.: Condens. Matter **20** (2008) 304212 (6pp) doi:10.1088/0953-8984/20/30/304212

Towards a simulation of disordered systems with interactions

Angus MacKinnon

Blackett Laboratory, Imperial College London, South Kensington campus, London SW7 2AZ, UK

E-mail: a.mackinnon@imperial.ac.uk

Received 7 January 2008
Published 8 July 2008
Online at stacks.iop.org/JPhysCM/20/304212

Abstract

We consider the problem of Anderson localization in disordered systems with interactions. We present a numerical approach in quasi-one-dimensional (quasi-1D) systems which combines aspects of the transfer matrix and Green's function recursion methods with the density matrix renormalization group. The method is applied to spinless fermions in 1D and a generalization to finite cross-sections is outlined.

1. Introduction

At least since the work of Anderson (1958), if not earlier (Landauer 1951), it has been known that the wavefunction in a disordered system can become localized and that this gives rise to a metal–insulator transition (MIT), either as disorder increases or as the Fermi level is changed. Much effort has been expended in numerical simulation of the non-interacting system, and a reasonable consensus has emerged, with theory and experiment in general qualitative agreement. Quantitative agreement, such as on the value of critical exponents or, even more difficult, the calculation of critical values of disorder or the Fermi energy in real systems, is a long way off. In three-dimensions (3D), for example, the calculated value of the critical exponent, assumed to be universal, is markedly larger than the experimentally measured value (Slevin and Ohtsuki 1999). This discrepancy would suggest that there is a fundamental problem either with the experiments and their interpretation or with the numerical work, or with both. An obvious factor missing from the numerical work is the electron–electron interactions. Furthermore, some have claimed to observe a metal–insulator transition in two-dimensions (2D), contrary to the widely accepted scaling theory of Anderson localization (Kravchenko *et al* 1994). This is often attributed to the effect of interactions. It is important therefore to consider the joint effect of disorder and interactions. Unfortunately, both aspects on their own constitute difficult problems. Combining them may well be considered over-ambitious. On the one hand, the model becomes a many-body system and the Hilbert space therefore grows exponentially with the system size. On the other hand, the simplifications which make the many-body problem at least partly tractable depend heavily on symmetry: something which cannot be applied to disordered systems. Nevertheless, there has been some progress which suggests that the inclusion of interactions may lead to non-trivial behaviour.

Shepelyansky (1994), for example, considered two interacting particles. In 1D, the interactions cause a large enhancement of the localization length. In 2D, Ortuño and Cuevas (1999) has presented evidence of an even stronger effect, possibly leading to delocalization.

For treating the finite density problem in an ordered system the most successful approach has been the density matrix renormalization group (DMRG) method (White 1992, 1993). This works by discarding basis states that do not contribute significantly to the ground-state density matrix. When this method was applied to the Anderson interacting model (defined in equation (1)), a delocalized regime was found for attractive interactions (Schmitteckert *et al* 1998, 1998a). Extensions of DMRG to 2D have encountered problems.

In trying to find an algorithm capable of dealing with the disordered and interacting systems, we have to overcome several difficulties. Firstly, most of the measures of localization used in the study of non-interacting systems are not easily applicable to many-body states. Secondly, the exponential growth of the Hilbert space must be tackled. This either requires us to reduce the number of states and keep the total within manageable bounds, or to define new quantities which encapsulate all the relevant information while remaining finite. Another possible approach would be to transform the system into an equivalent non-interacting one using a Hubbard–Stratonovich transformation or similar. This would

inevitably involve adding an extra dimension but is certainly something worth pursuing.

While searching for a suitable algorithm, certain facts of life have to be borne in mind. These tend to affect both the size of the storage requirements and the time required. Firstly, the time required to diagonalize a general $N \times N$ matrix scales as N^3. Thus, on both storage and time grounds, there is a clear preference for diagonalizing many small matrices rather than one large one.

Recent studies of non-interacting systems (Slevin and Ohtsuki 1999) have shown that, in order for the finite-size scaling analysis to be successful and reliable, the localization length must be calculated to better than 0.1% accuracy. Comparing this with the statistical behaviour of non-interacting systems implies that we require a length $L_{\max} = 10^6 \lambda_{\mathrm{M}}$, where λ_{M} is the localization length or, equivalently, a transmission coefficient $T = 10^{-868\,589}$. Note that this is much less than the machine accuracy, typically 2.2×10^{-16}. Hence any algorithm which requires us to calculate this quantity directly, rather than its logarithm, is likely to fail.

We, Carter and MacKinnon (2005), have developed a new approach incorporating aspects of DMRG together with the transfer matrix and Green's function recursion methods that have proved so successful for studying the non-interacting case (Carter 2003, MacKinnon and Kramer 1981, 1983). In this paper we will discuss an improvement on that method and a generalization to finite cross-section. We will also make some effort to relate this approach to Green's function recursion.

2. The algorithm

We start with a tight-binding model. The algorithm may be applied to any 1D or quasi-1D system, where the interactions are between nearest neighbours only. We should not expect, therefore, to describe phenomena, such as the Coulomb glass (Efros and Shkloviskii 1975), which are connected to long-range interactions.

2.1. Hamiltonians

The method can deal with a wide range of different Hamiltonians describing both fermions and bosons, with and without spin, such as

$$\hat{H}_{\mathrm{spinless}} = \sum_i \varepsilon_i \hat{c}_i^\dagger \hat{c}_i + V \sum_{i,j(n.n)} \left(\hat{c}_i^\dagger \hat{c}_j + \hat{c}_j^\dagger \hat{c}_i\right) + U \sum_{i,j(n.n.)} \left(\hat{c}_i^\dagger \hat{c}_i\right)\left(\hat{c}_j^\dagger \hat{c}_j\right) - \mu \sum_i \hat{c}_i^\dagger \hat{c}_i \tag{1}$$

$$\hat{H}_{\mathrm{Hubbard}} = \sum_{i\sigma} \varepsilon_i \hat{c}_{i\sigma}^\dagger \hat{c}_{i\sigma} + V \sum_{i,j(n.n),\sigma} \left(\hat{c}_{i\sigma}^\dagger \hat{c}_{j\sigma} + \hat{c}_{j\sigma}^\dagger \hat{c}_{i\sigma}\right) + U \sum_i \left(\hat{c}_{i+}^\dagger \hat{c}_{i+}\right)\left(\hat{c}_{i-}^\dagger \hat{c}_{i-}\right) - \mu \sum_{i\sigma} \hat{c}_{i\sigma}^\dagger \hat{c}_{i\sigma} \tag{2}$$

$$\hat{H}_{\mathrm{boson}} = \sum_i \varepsilon_i \hat{c}_i^\dagger \hat{c}_i + V \sum_{i,j(n.n)} \left(\hat{c}_i^\dagger \hat{c}_i + \hat{c}_i^\dagger \hat{c}_i\right) + U \sum_i \left(\hat{c}_i^\dagger \hat{c}_i\right)\left(\hat{c}_i^\dagger \hat{c}_i - 1\right) - \mu \sum_i \hat{c}_i^\dagger \hat{c}_i \tag{3}$$

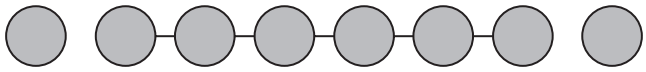

Figure 1. At each iteration a new site is added to both ends of a 1D chain.

which represent spinless fermions (1), the Hubbard model (2) and bosons (3), respectively. $\hat{c}_i^\dagger$ and $\hat{c}_i$ represent particle creation and annihilation operators. The first two terms constitute the standard Anderson (1958) model used widely in the study of the MIT. The extra U term represents the interactions, while the term in the chemical potential μ must be included, as the changing system size requires us to use a grand canonical ensemble. The chemical potential or Fermi energy μ controls the particle density in the system. If $U > 0$ the interactions are normal, that is, repulsive, whereas if $U < 0$ they are attractive. In common with most numerical studies of Anderson localization, we will work at temperature $T = 0$.

2.2. The recursive method

The original version of our algorithm (Carter 2003, Carter and MacKinnon 2005) required us to extend an existing chain by adding an extra site to both ends (figure 1).

At each step we consider a set of states which may be subdivided as

$$\begin{bmatrix} |0_1 \Psi^{L,N} \quad 0_L\rangle \\ |1_1 \Psi^{L,N-1} 0_L\rangle \\ |0_1 \Psi^{L,N-1} 1_L\rangle \\ |1_1 \Psi^{L,N-2} 1_L\rangle \end{bmatrix} \equiv \begin{bmatrix} \Psi_{00}^{L+2,N} \\ \Psi_{10}^{L+2,N} \\ \Psi_{01}^{L+2,N} \\ \Psi_{11}^{L+2,N} \end{bmatrix} \tag{4}$$

where $\Psi^{L,N}$ represents a state of a system of length L containing N electrons. The simplest representation is as a vector made up of four distinct parts, depending on whether the additional sites are occupied or unoccupied. Note that the subvectors Ψ_{10} and Ψ_{01} have the same length, as they include the same set of states with $N-1$ electrons. We can represent the subvectors using an alternative notation

$$\begin{aligned} \Psi_{00}^{L,N} &= \hat{c}_1 \hat{c}_1^\dagger \hat{c}_L \hat{c}_L^\dagger \Psi^{L,N} \\ \Psi_{10}^{L,N} &= \hat{c}_1^\dagger \hat{c}_1 \hat{c}_L \hat{c}_L^\dagger \Psi^{L,N} \\ \Psi_{01}^{L,N} &= \hat{c}_1 \hat{c}_1^\dagger \hat{c}_L^\dagger \hat{c}_L \Psi^{L,N} \\ \Psi_{11}^{L,N} &= \hat{c}_1^\dagger \hat{c}_1 \hat{c}_L^\dagger \hat{c}_L \Psi^{L,N} \end{aligned} \tag{5}$$

where we have used the fact that operating with $\hat{c}_n^\dagger \hat{c}_n$ on any vector filters out the subvector containing states in which site n is occupied, whereas $\hat{c}_n \hat{c}_n^\dagger$ does the same for the subvector in which site n is unoccupied. We note in passing that these combinations of operators could be rewritten as two-particle Green's functions.

Starting from this representation, a density matrix

$$\rho\,(1\ldots0, 0\ldots1) = \left\langle \Psi_{10}^{L,N} \middle| \Psi_{01}^{L,N} \right\rangle \tag{6}$$

$$\equiv \left\langle \Psi^{L,N} \middle| \hat{c}_1^\dagger \hat{c}_L \middle| \Psi^{L,N} \right\rangle \tag{7}$$

may be defined. This may be interpreted as the probability that the addition of an electron on the left results in an electron being emitted from the right. Again, we have a quantity which may be written in terms of a Green's function, but this time it is a single-particle 'lesser' Green's function, $G^<(1, L)$. The quantity may also be related to the dependence on boundary conditions (Schmitteckert *et al* 1998b, Kramer and MacKinnon 1993, Carter 2003). Note that, due to the indistinguishability of the electrons, it is meaningless to demand that the same electron emerges on the right. In fact, it is also valid classically to ask the question whether an electron emerges from the right whenever one is inserted on the left.

We can now define a localization length, λ_M, from

$$\rho(1\ldots0, 0\ldots1) \sim \exp(-2L/\lambda_M) \tag{8}$$

$$\Rightarrow \lambda_M = -\lim_{L\to\infty} \frac{2L}{\ln \rho}. \tag{9}$$

This is very similar to the definition used in transfer matrix calculations and is closely related to the sensitivity to boundary conditions (Carter 2003).

2.3. Reducing the Hilbert space

A tractable algorithm for an interacting system must deal with the exponential growth of the Hilbert space. It would clearly be preferable to find a quantity whose dimensions do not increase and which nevertheless encapsulates all the information required, but, pending such a breakthrough, we are obliged to find a strategy for throwing away states. Within the tight–binding framework it is the only approximation in our method.

In general we expect to find that a simple energy cutoff will lead to the retention of the lowest energy states for a range of particle numbers, N, around the desired density. As a first attempt (Carter 2003, Carter and MacKinnon 2005) we tried to choose a cutoff energy by fixing a maximum matrix size and then applying that cutoff to all states. This tended to result in the retention of those states with $N_{\min} \pm 4$, where $N_{\min}$ is the number of particles for the state with the lowest grand canonical energy; those for other particle numbers have ground states above the energy cutoff. Unfortunately, we found that this simple criterion failed to result in exponentially decaying behaviour of $\rho(1\ldots0, 0\ldots1)$, even in the absence of interactions. Hence it failed the simplest test for any sensible approach to our problem: that it correctly reproduces the expected behaviour for non-interacting disordered systems.

We later realized that fixing an energy cutoff but allowing the number of retained states to fluctuate produced better results, and this is the criterion we used in all subsequent work using this model. We note that this can potentially lead to difficulties with very large matrices. It also involves an implicit assumption about the nature of the distribution of many-body states close to the ground state; namely, that the density of low-lying states reaches some sort of equilibrium for long system sizes. While this assumption is consistent with the results of our calculations, it remains unclear whether this is a true property of the system or an artefact associated with the cutoff process itself.

Experience with DMRG (White 1992) suggests that a more sophisticated cutoff method is required and that a simple energy cutoff, such as we have used, is too naïve.

3. The spinless single chain

3.1. Non-interacting limit

As the localization properties of a one-dimensional non-interacting chain are well established (Pendry 1982a, 1982b, 1986, 1987, Pendry and Kirkman 1984, 1986, Pendry *et al* 1986, Slevin and Pendry 1988, Pendry and Barnes 1989) this case serves as a simple test of the effectiveness of any algorithm which aims to study the more complex problem. All eigenstates are localized for any amount of disorder with a localization length which depends on disorder as quoted as (Kramer and MacKinnon 1993)

$$\lambda^{-1} = \frac{W^2}{24(4V^2 - \mu^2)}. \tag{10}$$

This is only valid for small disorder and there are numerous special cases, but it is sufficiently general to serve as a test in the present case. Note that the localization length diverges in the limit of small disorder.

3.2. Clean phase space

The second limiting case is that of zero disorder with interactions. This case can be mapped onto an XXZ spin chain model and solved exactly for half-filling (Pang *et al* 1993, Yang and Yang 1966a, 1966b, 1966c).

There are two limiting cases. For large positive U, repulsive interactions, a charge density wave (CDW) is found in which alternate sites are occupied. On the other hand, for attractive interactions and $0 > U > -2$, the interaction tends to cause clustering, but this is offset by the kinetic energy which tends to spread the particles. This reaches an extreme form for $U < -2$ when the lowest grand canonical energy corresponds to either a completely full or a completely empty system. Here we expect to see phase separation or domain formation. This can be seen in figure 2. Note the increasingly well defined minimum at half-filling with increasing positive U and the maximum for $U < -2$. As the $U = -2$ limit is reached from above, the ground-state energy becomes independent of particle number N; the compressibility diverges. Above $U = +2$, a charge gap opens up (Pang *et al* 1993, Bouzerar and Poilblanc 1994) and the CDW corresponds to a Mott insulator state.

3.3. Typical results

As an illustration of the sort of results obtained with this method in the non-interacting limit, consider figure 3. The effect of interactions is shown in figure 4. Neither figure is wholly satisfactory: the agreement with known results (figure 3) is qualitatively correct, but there are clearly quantitative differences. The number of retained states is still too much of a factor (figure 4). Although the results appear to be a long way from convergence, the qualitative behaviour is as expected.

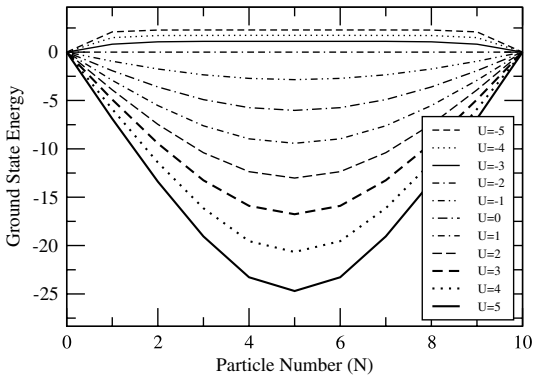

Figure 2. Grand canonical ground-state energy for a (clean) chain of ten sites as a function of particle number, N. The chemical potential is chosen for half-filling (i.e. $\mu = U$).

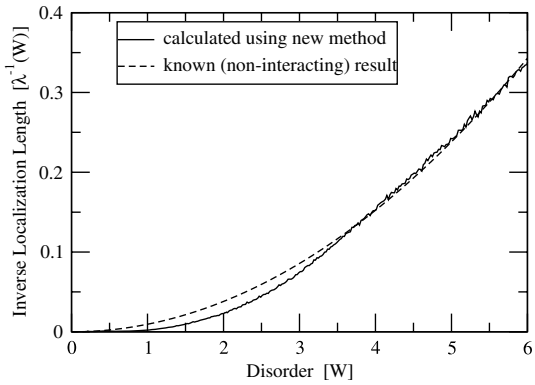

Figure 3. Inverse localization length against disorder when interactions are turned off. The dotted line corresponds to (10). The continuous line shows results for systems of up to 1000 sites, with 480 basis states on average retained per iteration. The results were averaged over 1000 disorder realizations.

3.4. Problems with the original algorithm

The other fundamental difficulty with the original form of the algorithm, besides the number of retained states, is the necessity to calculate the scalar product in (7). This cannot be calculated when its value drops below the machine accuracy, 2.2×10^{-16}. This in turn limits the tractable length to below $L = 1000$. The statistical issues this raises may be overcome by averaging over smaller systems, but this is only useful if there are no other length scales in the problem which are comparable with or larger than $L = 1000$.

The calculation fails for low disorder, $W/V = 2$ ($-\frac{1}{2}W < \epsilon < +\frac{1}{2}W$), even for $U = 0$. In this regime the density matrix does not fall exponentially but tends to saturate at a finite value.

At each stage 75% of the states are eliminated. It is not clear whether this really constitutes a problem. In any case this is probably related to the fact that the convergence with the number of retained states is unsatisfactory. The situation improves when an energy cutoff is used and the number of states is allowed to fluctuate, but convergence remains unacceptable.

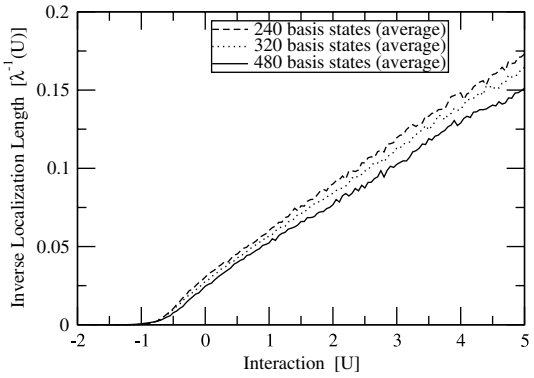

Figure 4. Inverse localization length as a function of U. The three lines correspond to different energy cutoff values. Each line is averaged over 1000 systems which are allowed to extend to a maximum of 1000 lattice sites. Disorder $W = 2$.

4. An improved algorithm

Let us start from the density matrix (7) written in the site-occupation basis

$$\rho\,(1\ldots0,0\ldots1) = \mathrm{Tr}\left[\mathbf{U}^{(L,N)\dagger}\hat{c}_1^\dagger\mathbf{U}^{(L,N-1)}\hat{c}_L\right] \tag{11}$$

where $\mathbf{U}^{(L,N)}$ is the $(2^L \times K^{(L,N)})$ matrix whose columns are the $K^{(L,N)}$ retained states. We now define a new matrix

$$\mathbf{P}^{(L,N)} = \mathbf{U}^{(L,N)\dagger}\hat{c}_1^\dagger\mathbf{U}^{(L,N-1)} \tag{12}$$

which may be interpreted as a representation of the operator $\hat{c}_1^\dagger$ in the reduced Hilbert space. $\mathbf{P}$ obeys the recursion relation

$$\mathbf{P}^{(L+1,N)} = \mathbf{V}^{(L+1,N)\dagger}\begin{bmatrix}\mathbf{P}^{(L,N)} & \mathbf{0}\\ \mathbf{0} & \mathbf{P}^{(L,N-1)}\end{bmatrix}\mathbf{V}^{(L+1,N-1)} \tag{13}$$

in which $\mathbf{V}^{(L+1,N)}$ is the matrix which transforms the eigenvectors for a system of length L with N electrons into those of a system of length $L+1$ such that

$$\mathbf{U}^{(L+1,N)} = \begin{bmatrix}\mathbf{U}^{(L,N)} & \mathbf{0}\\ \mathbf{0} & \mathbf{U}^{(L,N-1)}\end{bmatrix}\mathbf{V}^{(L+1,N)}. \tag{14}$$

Using $\mathbf{P}$ we are able to calculate the required density matrix, $\rho = \mathrm{Tr}[\mathbf{P}^{(L,N)}\hat{c}_L]$, and hence the localization length, while only adding a site to one end. In this case we only throw away 50% of the states at each iteration, rather than the previous 75%. Use of the matrix $\mathbf{P}$ brings an unexpected and far more important bonus. Equation (13) has a product structure which never requires us to calculate a scalar product of two almost orthogonal vectors. It is thus possible to calculate $\mathbf{P}$, and hence ρ, accurately even when its value drops many orders of magnitude below the machine accuracy. In fact we can employ the same tricks as are used in transfer matrix calculations so that we do not even run into the minimum representable number. Other problems with the algorithm also disappear: the method now behaves sensibly for low disorder and for values of U approaching the limit at $U \to -2$. In fact there are no remaining restrictions on the parameter ranges for which the

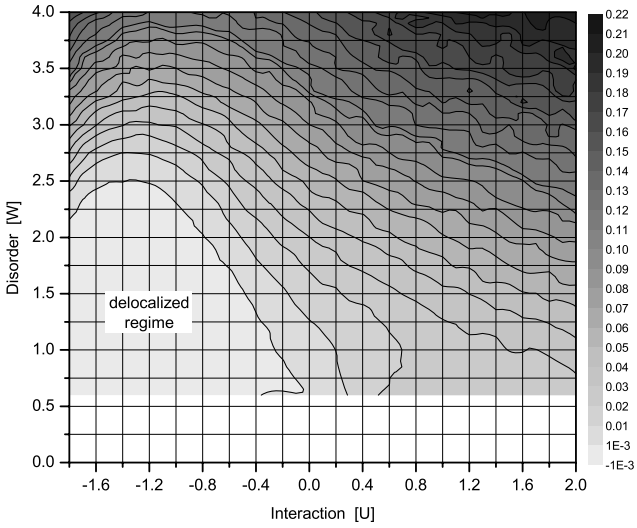

Figure 5. Disorder-interaction phase space plot for the single chain spinless model at half-filling. The contours represent the inverse localization length in intervals of 0.01. The lowest interval corresponds to a localization length greater than 1000 sites. This plot was produced using over 1300 points. Each point was averaged over 250 systems in which chains were allowed to extend to 2000 sites and approximately 240 basis states were retained per iteration. Data for $W < 0.6$ is not shown because the method is unreliable for low disorder.

method behaves sensibly (other than $U < -2$). An additional bonus is that exponential behaviour is obtained irrespective of the method used for throwing away states. This should not be too much of a surprise, as such behaviour is an almost inevitable consequence of the product structure mentioned above. All this suggests that the earlier results were heavily influenced by the presence of a second length scale which may have been larger than the largest system sizes attainable.

4.1. Disorder-interaction phase space

Figure 5 summarizes the results obtained with the original algorithm and which we aim to improve with the new method. Results for low values of W/V are not available and the delocalized region comes too close to $U = 0$. We are now able to fill out the gaps in this diagram and even more reliably to study the boundary of the extended regime. It should also be possible to extract information about the critical behaviour. This is, however, a longer-term undertaking.

Nevertheless, the data in figure 5 contain many more points than in previous work and refer to significantly larger samples (Bouzerar and Poilblanc 1994, Schmitteckert and Eckern 1996, Schmitteckert *et al* 1998b, 1998, Weinmann *et al* 2001). It should be noted that the upper limit of the delocalized regime around $W = 2.5$ is a factor of two higher than predicted by Schmitteckert *et al*, but lower than in earlier work (Bouzerar and Poilblanc 1994).

5. Generalization to a finite cross-section

In our first attempts to deal with systems of width two or with the Hubbard model (Carter 2003) we added a complete slice or atom at each iteration. While this may be made to work for small systems, it rapidly becomes prohibitively expensive and, beyond a relatively small cross section, $M = 8$, completely intractable. Instead we consider a method by which additional sites are added to the $L \times M$ system one at a time. In order to do so it is necessary to define a set of new ancillary matrices which are designed to retain the information required to add subsequent atoms to the slice. These are

$$\mathbf{Q}_m^{(L,N)} = \mathbf{U}^{(L,N)\dagger} \hat{c}_m^\dagger \hat{c}_m \mathbf{U}^{(L,N)} \tag{15}$$

$$\mathbf{R}_m^{(L,N)} = \mathbf{U}^{(L,N)\dagger} \hat{c}_m^\dagger \mathbf{U}^{(L,N-1)}, \tag{16}$$

which may be interpreted as representations of the number operator and creation operator, respectively. $\mathbf{Q}$ is required for

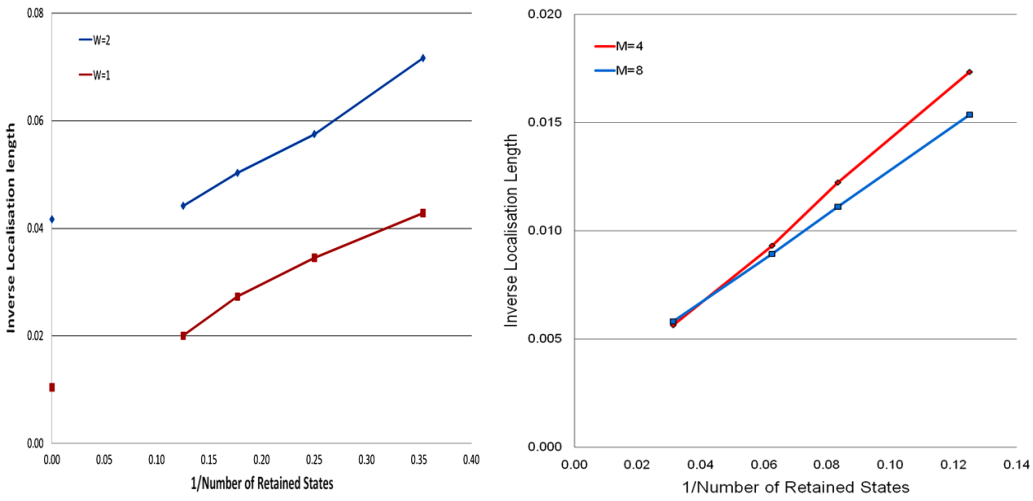

Figure 6. The inverse localization length for $U = 0$ and $W = 1$ and 2 in 1D (left) and for strips of width $M = 4$ and 8 (right) plotted against the inverse of the number of retained states. The dots on the left-hand axis (left-hand figure) indicate the known results for the non-interacting system.

(This figure is in colour only in the electronic version)

calculating any interaction terms involving a new site and site m, whereas **R** is required for the corresponding hopping terms.

Both **Q** and **R** may be updated recursively in a similar way to **P**, and their size is that of the number of retained states.

6. Convergence

While we have now made significant progress in overcoming some of the problems which plagued our initial attempts to study disorder and interactions, it must be conceded that one major difficulty remains. This is illustrated in figure 6. Here we see that the convergence with the number of retained states is far from satisfactory. In order to improve this we aim to learn from DMRG (White 1998), even if previous attempts at direct use of that method left much to be desired. We also note the interesting relationship between the ancillary quantities required to improve the algorithm and various Green's functions. This is also a promising avenue for further work.

6.1. Summary

We have presented a method of studying disordered and interacting quasi-one-dimensional systems which combines aspects of the transfer matrix and DMRG approaches. We have been able to overcome some of the difficulties encountered in our earlier method, and are now able to study systems significantly larger than those achieved hitherto. However, there is still room for improvement. In particular, it is important to develop a more effective strategy for reducing the Hilbert space, either by throwing away states or by defining new quantities which encapsulate all the required information.

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