Disorder and interactions in one-dimensional systems

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We present a numerical approach to the study of disorder and interactions in quasi-one-dimensional (1D) systems which combines aspects of the transfer matrix method and the density matrix renormalization group which have been successfully applied to disorder and interacting problems, respectively. The method is applied to spinless fermions in 1D, and the existence of a conducting state is demonstrated in the presence of attractive interactions.

I. INTRODUCTION

It is well established that in the presence of disorder electron wave functions can become localized. Considerable numerical work has been carried out for noninteracting systems, with results reaching a reasonable consensus: theory and experiment are in general qualitative agreement. However, in 3D the calculated value of the universal critical exponent is markedly larger than the experimentally measured value. This seems to suggest that an essential factor is missing from calculations: the obvious candidate is the electron-electron interaction. Furthermore, some have claimed to observe a metal-insulator transition in 2D contrary to the widely accepted scaling theory of Anderson localization. This is often accredited to the effect of interactions. Hence, during the last 10 years attention has been switching to this more difficult case. The central problem is that the model becomes a many-body system and so the Hilbert space grows quickly with system size. This renders an exact numerical calculation far beyond computational capabilities. Nevertheless, several studies have been accomplished; these suggest inclusion of interactions may yield nontrivial behavior.

Shepelyansky performed calculations on two interacting particles. In 1D, interactions caused a large enhancement of localization length. Other work showed that in 2D the effect is possibly stronger, leading to delocalization. However, some caution is required as the method fails to reproduce known noninteracting results when interactions are switched off.

The most successful method for treating the finite density problem is the density matrix renormalization group (DMRG) approach. This works by performing a direct diagonalization but reducing the Hilbert space by systematically discarding basis states that do not contribute significantly to the ground state. Applying this method to the Anderson interacting model [defined in Eq. (1)], a delocalized regime was found for attractive interactions. In more recent papers by the same authors, it was noted that interesting physics is washed out in the averaging process. Charge reorganizations can be seen as electrons on a chain shift from the Mott insulator limit (strong interactions) to the Anderson insulator limit (strong disorder). Extensions of DMRG to 2D have encountered difficulties.

We have developed a method incorporating some of the ideas of DMRG and the transfer matrix method successfully used in the noninteracting case. Section II describes the method and Sec. III discusses the application to a model of spinless fermions.

II. THE NEW METHOD

Like DMRG and the usual transfer matrix, our approach is based on a tight-binding model. It can be readily applied to describe any 1D or quasi-1D system, provided interactions are nearest neighbor.

A. The Hamiltonian

The Hamiltonian for spinless fermions may be written in terms of particle creation \( \hat{c}_i^+ \) and annihilation \( \hat{c}_i \) operators for site \( i \)

\[
\hat{H} = \sum_i e_i \hat{c}_i^+ \hat{c}_i + V \sum_i (\hat{c}_i^+ \hat{c}_{i+1} + \text{H.c.}) + U \sum_i (\hat{c}_i^+ \hat{c}_{i+1} \hat{c}_{i+1}^* \hat{c}_i^* + \text{H.c.}) - \mu \sum_i \hat{c}_i^+ \hat{c}_i.
\]

The first two terms constitute the standard Anderson model used widely in the study of disorder-induced localization. The additional \( U \) term represents the nearest-neighbor interaction. If neighboring sites are occupied then the two particles experience a repulsive \( (U>0) \) or possibly attractive \( (U<0) \) force. \( U=0 \) corresponds to the noninteracting case.

The final term represents the chemical potential \( \mu \). This must be included as the method works within the grand canonical scheme in which a range of particle numbers will be considered. The value of the parameter \( \mu \) controls the particle density of the system. As with most numerical studies of Anderson localization, zero temperature will be assumed.

B. The recursive method

In common with other approaches to the many-body problem, we tackle the issue of the exponentially growing Hilbert space by reducing the number of basis states, restricting the focus to the ground state. This works in conjunction with a recursive procedure that extends the chain by successively adding new sites. Open boundary conditions must be used.
For each iteration:

(1) A site is added to each end of the chain (Fig. 1) and basis states are constructed. At first sight it may appear simpler to add a new site to one end only. However, it turns out that for the purposes of measuring the degree of localization it is much more natural to add sites to both ends of the chain in the same iteration (Sec. II C).

(2) For each particle number with remaining basis states a Hamiltonian matrix is found. After the matrix elements have been calculated, the Hamiltonian is solved and the desired quantities are extracted.

(3) Finally, a proportion of the resulting eigenstates are thrown away according to some criterion. The remaining states are used to form the basis at the next iteration—a chain with two more sites.

There is no fundamental reason why this process cannot be repeated to very large chain lengths. The following sections detail the mathematics of this procedure.

1. Expressing the basis states

For a one-dimensional chain, with $L$ sites and one electron per site, there are $2^L$ basis states. In order to reduce the Hilbert space, this method relies on the fact that it is possible to express the states for a chain of length $L$ in terms of the energy eigenstates $|\Phi^{\ell-2}\rangle$ of the chain of length $L-2$ (i.e., the same chain without the two end sites). Thus, for every eigenstate $|\Phi^{\ell-2}\rangle$ of the $L-2$ site chain, there are four corresponding basis states for the $L$ chain: $|0\Phi^{\ell-2}\rangle, |1\Phi^{\ell-2}\rangle, |0\Phi^{\ell-2,1}\rangle$, and $|1\Phi^{\ell-2,1}\rangle$.

Consequently, a general state for the $L$ chain with $N$ electrons, $|\Psi^{L,N}\rangle$, may be written as a linear combination of basis states in the following manner:

$$|\Psi^{L,N}_{m,n}\rangle = \sum_i a_{mn} |0\Phi^{L-2,N}_{0}\rangle + \sum_j b_{nj} |1\Phi^{L-2,N-1}_{0}\rangle + c_{nj} |0\Phi^{L-2,N-1}_{1}\rangle + \sum_k d_{nk} |1\Phi^{L-2,N-1}_{k}\rangle. \quad (2)$$

In fact, as the number of electrons is a good quantum number, it is only necessary to consider the subset of $|\Phi^{\ell-2}\rangle$ states which, when combined with two new end sites, have a total of $N$ electrons.

2. Calculating the Hamiltonian matrix

A separate Hamiltonian can be calculated for each value of $N$. In order to do so, we have to express the eigenfunctions in a basis in which the final states are clearly either occupied or unoccupied. This can be accomplished by first expanding each of the four types of basis states back a further generation, in terms of the previous iteration $|\Phi^{\ell-1}\rangle$.

\[ |m\Phi^N_i\rangle = \sum_p a^{mn}_{ip} |0\Phi^N_p\rangle + \sum_q b^{mn}_{iq} |1\Phi^N_{q-1}\rangle + c^{mn}_{ir} |0\Phi^N_{r-1}\rangle + \sum_s d^{mn}_{is} |1\Phi^N_{s-2}\rangle, \quad (3) \]

where $m,n=0,1$, and the $L-4$ superscripts have been dropped for the sake of clarity. This Hamiltonian can be diagonalized for each value of $N$ and the corresponding ground state found. The overall ground state is then found by comparing the values for different $N$.

3. Reducing the number of basis states

The purpose of reformulating the basis states and in turn the Hamiltonian in this manner is to enable an approximation to be introduced which keeps the dimension of the Hilbert space roughly constant as sites are added. During each iteration a proportion of the basis states must be thrown away according to some systematic method. This is necessary to keep the calculation to a computationally manageable size. Within the tight-binding framework, it is the only approximation in our method.

There are several possible schemes which could be used. A criterion is required that produces the smallest error on the next iteration ground state, as it is the properties of the ground state, which are of interest. Naively, the lowest energy states could be kept. More sophisticated approaches would determine which states make the largest contribution to the next iteration ground state. Whichever method is adopted, some justification will be required as will the determination of the limits of its accuracy.

The simplest method to implement is to throw away the states of highest energy, so this will be adopted initially. We choose the size, $M$, of the largest matrix we will tolerate and introduce a common energy cutoff for all $N$ such that the largest number of retained states for any $N$ is $M$. The value of $M$ can be changed to control the accuracy where higher accuracy of course entails larger processing time and memory requirements. In practice, only states for a small range of $N (<10)$ around the ground state are retained by this procedure.

C. Measuring the localization length

The aim of this new method is to understand the effect of varying system parameters, in particular the interaction strength $U$, on electron localization. For noninteracting systems several measures of localization have been developed, most of which cannot be simply carried across into the many-body case. It is worth noting that these measures are not all equivalent in that they tend to give different statistical weight to different aspects of the system. Although they all tend to reveal the same trends in behavior, they are often quantitatively different. Hence, simplistic comparisons between different measures of localization can be misleading.

One measure which is applicable to both interacting and noninteracting systems is the sensitivity to boundary conditions (BCs). The boundary conditions in a ring system
are changed from periodic to antiperiodic, and the changes in
energy measured. These changes may be interpreted as a
measure of the group velocity in the system and hence as a
measure of localization. However, although we can define
this quantity for both interacting and noninteracting systems,
the energies involved are different and cannot be directly
compared.

In our case, however, we do not have a ring. In principle
we could introduce a matrix element between the two ends,
diagonalize the system again, twice, and compare the results.
We have done so as a test but the results are consistent with
a much less computationally intensive procedure. Instead, we
introduce a small matrix element as a perturbation and cal-
culate the resulting energy change. This may be expressed in
terms of the off-diagonal elements of the reduced density
matrix between the two end sites

$$D = \rho_{\{i-1\} \{0\} \{0\} \{i+1\}} = \rho_{\{0\} \{i-1\} \{i\} \{0\}} = \sum_j b_{0j} c_{0j},$$

(4)

where $b_{0j}$ and $c_{0j}$ are the components of the ground-state
eigenfunction as defined in (2).

D. Computational implementation

The structure of the central algorithm is shown in Fig. 2.
To extract sensible data, localization quantities must be
averaged over many systems. Conventional practice is to
perform a geometric average which is achieved by averaging
the logarithm of the reduced density matrix (4). Then, least-
square fits were carried out to extract the localization length
over a minimum of ten sites. A couple of minor modifications
were made to the procedure as described. These were
necessary to cope with rare events.

(1) At least one state was retained for all values of $N$
within the range of $N$ for which there were eigenstates below
the energy cutoff. Otherwise, intermediate values of $N$ could
be eliminated, causing unnecessary complications in the pro-
gramming.

(2) At least three values of $N$ were always retained, to
avoid the phase space collapsing and the system, in effect,
being stuck in a local minimum.

Further details of the actual implementation of the method
can be found in the Ph.D. thesis of one of the current
authors.9

III. THE SINGLE-CHAIN MODEL

The method was first applied to the Hamiltonian (1)
modified to ensure particle-hole symmetry around $\mu=0$:

$$\hat{H} = \sum_{i=1}^{L} (e_i - U) \hat{c}_i^{\dagger} \hat{c}_i + V \sum_{i=1}^{L-1} (\hat{c}_i^{\dagger} \hat{c}_{i+1} + \hat{c}_{i+1}^{\dagger} \hat{c}_i) + U \sum_{i=1}^{L-1} (\hat{c}_i^{\dagger} \hat{c}_{i+1}^{\dagger} + \hat{c}_{i+1} \hat{c}_i)$$

$$\times (\hat{c}_{i+1}^{\dagger} \hat{c}_i + \hat{c}_i^{\dagger} \hat{c}_{i+1}) + \frac{U}{2} \hat{c}_1^{\dagger} \hat{c}_1 + \frac{U}{2} \hat{c}_L^{\dagger} \hat{c}_L - \mu \sum_{i=1}^{L} \hat{c}_i^{\dagger} \hat{c}_i.$$

(5)

This is the conventional 1D Anderson model with nearest-
neighbor interactions. We set $V=1$ (hence defining the
energy scale for both $U$ and $W$). The following two subsections
outline some useful features already known about this model
in two limits: no interactions ($U=0$) and no disorder ($W$
=0).

A. Noninteracting behavior

The localization properties of a one-dimensional noninter-
acting chain are well established. For any amount of disorder
all eigenstates are localized. The dependence of localization
length on disorder is usually quoted as13

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

(6)

This is only valid for small disorder. Note that the localiza-
tion length diverges in the clean limit. Therefore, an impor-
tant test for the new recursive method is to reproduce this
behavior. However, care is required in making the correct
comparison: how does this dependence carry across from
the single-particle case to the many-particle case?

B. Clean phase space

The second limit to be outlined is the zero-disorder phase
space. Without randomness the present model can be mapped
to an XXZ spin-chain model and solved exactly for
half-filling.15–18

A program was constructed to perform exact diagonaliza-
tions on short chains in order to compare results. This was
necessary because the method under development does not
use the particle occupation basis. The computational limit is
about ten sites, but nevertheless gives valuable insight into
the nature of the ground state for different regions of phase
space.

At half-filling there are two limiting forms of the ground
state with a crossover regime. For large repulsive interac-
tions a charge density wave (CDW) is observed (i.e., alter-
FIG. 3. Results from a (clean) short chain of ten sites demonstrating phase separation for $U<−2$. For each particle number the (grand canonical) ground-state energy is plotted. The chemical potential is set to give half-filling as the overall ground state (i.e., $\mu=U$). Plotted energies are grand canonical.

short chains it is not possible to pinpoint where this gap above this point corresponds to a Mott insulator state. For order destroys the charge gap and long-range order associating with it. The authors conclude that even weak dis-\(t\)ential is set to give half-filling as the overall ground state/\(h\)strating phase separation for paper/\(h\)19 performs exact diagonalizations on small systems and in particular, to map out the delocalized regime. One paper/\(h\) and Schulz,20 although they acknowledge an earlier paper.21

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Numerical work has sought to verify these predictions, and in particular, to map out the delocalized regime. One paper/\(h\)19 performs exact diagonalizations on small systems (up to 22 sites). The results are consistent with the expected delocalized phase, although the chain length is so small they cannot exclude the possibility that the localization length is very large.

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FIG. 4. The average of $\frac{1}{2} \ln(D^2)$ as a function of chain length \(L\), where \(D\) is the reduced density matrix (4). Averages are geometric, that is, the mean of $\ln(D^2)$ is found. The chain length is allowed to extend until numerical precision is lost. The $\mu=0$ case was stopped at 20,000 sites as it had saturated long before. System parameters are \(W=2\), \(U=0\), and the energy cutoff is set using \(M=10\) (corresponding to a total of approximately 160 basis states per iteration). The averages were taken over 2000 systems.

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The most extensive work has been conducted by Schmitteckert et al. applying DMRG to both the interacting Anderson model and to the related problem of persistent currents in mesoscopic rings.7,14,22,23 The first study examining Anderson localization/\(h\)14 was on chains extending up to 60 lattice sites. The degree of localization was measured by the phase sensitivity to boundary conditions. Two regimes were found: a localized phase, \(U>−1\), and delocalized regime, \(U<−1\), consistent with work already mentioned. In fact, it was found that repulsive interactions increase localization. After considerable numerical effort a phase diagram was produced, showing where the two regions lie in disorder-interaction space. The authors believe the earlier attempt/\(h\)19 based on an RG procedure overestimates the delocalized regime by a factor of 4. Other authors, Römer24 and Schuster et al.,25 have mapped out an extended regime for the same model but with the Aubry-André quasiperiodic potential. However, its shape in disorder-interaction phase space takes on a different form.

C. Previous work

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D. Determining limits and accuracy

We must first understand the broad behavior of the method before using it to determine specific results.

1. Determining numerical limits

Figure 4 shows some typical results where the chain length has been allowed to extend as far as possible. A range of values of $\mu$ was used, spread across the band (between $\mu=−2$ and $\mu=2$ in the noninteracting case). The lines pair up, with $\mu=−\mu'$ and $\mu=+\mu'$ giving near-identical results and thus demonstrating the anticipated symmetry in the band.
Straight lines indicate exponential localization, which is seen near the band edge. However, in the center of the band different behavior is observed: the curves show some form of decay which saturates at large chain lengths. Apart from the $\mu=0$ case, all simulations continued until numerical precision limits were reached. Off-diagonal elements of the reduced density matrix correspond to “scalar product”-type quantities (4). When the two vectors become almost perpendicular the product becomes very small. In this limit, numerical rounding dominates over the physics, rendering any results based on this regime meaningless. A criterion was devised to automatically halt simulations before this numerically inaccurate region is reached. This condition gives the upper length limit for linear fits which determine the inverse localization length. A lower limit was also set in which typically the first 20% of sites was ignored to allow the simulation to “settle down.”

2. Particle-hole symmetry test

The particle-hole symmetry test can be verified by looking at two chains using the same random distribution of site energies, but with one the negative of the other. On doing so, identical results are obtained. Thus, the electron-hole consistency test is convincingly satisfied.

3. Reducing the number of basis states (revisited)

The initial results (Fig. 4) show that the method fails in the middle of the band—exponential decay is not observed in the noninteracting case. This must be due to the Hilbert space reduction criterion, as it is the only approximation in the method. A simple variant on the original procedure was tried: the total number of states for all particle numbers was fixed rather than using a fixed number for the ground-state particle number only. This simple modification induced a significant change in the results. Although the decay was still nonexponential, this change clearly yields an improvement toward the expected behavior (Fig. 5).

Presumably the key difference between the methods is that using states from all particle numbers results in an energy cutoff which fluctuates less. Therefore, the natural criterion to try next is a fixed energy cutoff. This can be done by averaging the value of the cutoff using the fixed number of states method. Then, a fit of the cutoff as a function of chain length could be used as a fixed energy cutoff. It turns out that it is not possible to do this as an absolute cutoff because the ground-state energy fluctuates too much. However, it can successfully be done as a fixed energy cutoff relative to the ground state. When implemented, exponential decay is observed in the middle of the band (Fig. 5).

We conjecture that this dramatic improvement, resulting from an apparently innocuous change in cutoff methods, can be explained in terms of energy level statistics. Consider the middle of the band with no interactions: electrons should be localized, with states obeying Poisson statistics. One may envisage the system accidentally encountering a higher density of low-lying energy states. According to the original method, the energy cutoff is correspondingly lower. Thinking in terms of energy level repulsion, this would result in a release of “pressure” as a larger number of states are removed. The opposite scenario in which states accidentally spread wider than average may also be considered. In this case, the cutoff has a smaller effect than normal. The combined effect is to reduce fluctuations, causing the system to bear more resemblance to a Wigner distribution. In other words the system tends toward delocalization, consistent with the data in Fig. 5.

The second cutoff method implemented worked by fixing the cutoff using states across all particle numbers. According to the picture just outlined, the same effect of dampening fluctuations should still be present, although less severe because using a greater number of states reduces fluctuations of the cutoff energy. This can also be observed in Fig. 5, where the delocalizing effect is not so strong.

The third procedure for discarding states used a fixed energy cutoff, which is completely uncorrelated to the density of low-lying states. Therefore, the delocalizing effect is completely absent.

E. Comparison with noninteracting results

The new fixed energy cutoff may be used to provide further verification by checking that, when interactions are turned off, noninteracting results can be reproduced. This is particularly important as some well-established methods applied to the two-interacting particle model can fail in this respect (e.g., the transfer matrix method26,27).

1. Dependence on disorder

As a test of the accuracy of the method, Fig. 6 was produced. The calculated results should correspond roughly to the known result (6). Values are of the correct order of magnitude, but the new method does seem to give a dependence on $W$ greater than $W^2$. However, we should not expect exact correspondence as the two quantities are defined differently and intrinsically involve different statistical averages.
2. Convergence

Figure 7 illustrates the convergence of the method as the energy cutoff is raised. For $W=2$, the system is probably not converged for the largest number of retained states. For $W=5$ the convergence is much better. In fact, for very small $W$ the results are so sensitive to the cutoff that no meaningful pattern can be deduced.

One could consider proceeding by just examining interaction effects for $W>4$. However, interesting physics is expected when disorder, interactions, and the kinetic energy are of similar strength. Note that the standard deviation, $W/\sqrt{12}$, is a more satisfactory measure of disorder, so that this condition is fulfilled when $W=\sqrt{12}$ and $U=\pm 1$.

IV. RESULTS

Despite the unanswered questions, results were successfully obtained using the fixed energy cutoff procedure for eliminating states. The value for the cutoff was determined by first using the fixed number procedure for a small number of systems. When the average number of basis states is given, it refers to the number of basis states used with the fixed number procedure in order to determine the fixed energy cutoff. In addition, note that previous work by other authors focuses on the case of half-filling, so results presented in this section also examine this particle density.

A. Dependence on interaction strength

Of central interest is the effect of electron-electron interactions on localization. Figure 8 shows the calculated dependency for disorder $W=2$. Three different energy cutoffs were used corresponding to different numbers of retained states.

The overall behavior is unambiguous: repulsive interactions enhance the effect of disorder, whereas attractive interactions reduce it. For $U>0$ the inverse localization length increases with interaction strength. For $U<0$ the inverse localization length decreases with interaction strength.

FIG. 6. The dependence of inverse localization length on disorder when interactions are turned off. Results from the new method should correspond to known result for the middle of the band. Systems were allowed to extend up to 1000 sites, retaining an average of 480 basis states per iteration. Averages were taken over 1000 disorder realizations.

FIG. 7. The dependence of inverse localization length on the average number of basis states retained per iteration for the noninteracting case with disorder $W=2$ (a) and $W=5$ (b). The insets show this quantity plotted against the actual energy cutoff used. Such plots can be used to test for convergence. Data were averaged over 100 systems with chains extending up to 1000 sites.

FIG. 8. The dependence of localization length on interaction strength. 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 $W=2$. 
has an approximately linear relationship to interaction strength. Below $U = -1$ the localization length diverges. This apparently extended regime is anticipated from previous work (Sec. III C). Nevertheless, it remains possible that the system is localized but with a localization length in excess of the maximum system size. Unlike in three dimensions, there is no numerical signature which distinguishes between extended states and very large localized states. This has always been a particular problem in the weakly localized regime in two-dimensional systems. It can also be difficult to distinguish between truly extended states and power-law localized states or states with any sort of fractal structure. With this caveat we will refer to this regime as extended or delocalized.

Note that, due to the “flattening” effect (Fig. 3) toward the phase separation, the many-body density of states rises rapidly with energy. For a fixed energy cutoff this means that more states are retained over a greater range of particle numbers. This reduces computational performance and so the region $-2 < U < -1.8$ has not been explored. Data were obtained down to about $U = -1.8$ and are displayed in Fig. 8.

In higher dimensions we would proceed to try to calculate a critical exponent using a procedure such as finite size scaling.\textsuperscript{13} This is not directly applicable to the 1D system we are studying. In fact, it is not even clear that the localization length must diverge as a power law. Schmitteckert\textit{ et al.}\textsuperscript{14} argue that the exponent is nonuniversal. Nevertheless, a simple fit to the data in Fig. 8 for $U_c < U < 0$ gives $U_c = -1.375$ and $\nu = 3.0 \pm 0.4$. Hence, we can say that the data are at least consistent with a power-law divergence of the localization length.

B. Disorder-interaction phase space

Having confirmed the existence of a delocalized regime for attractive interactions, it was natural to attempt to map out the extent of this region. This was done in disorder-interaction phase space as plotted in Fig. 9. The area marked as delocalized corresponds to systems with a localization length greater than 1000 sites. If the number of systems averaged over were increased, then this criterion could be made more stringent. With this definition it can be seen that the delocalizing effect does not extend beyond $W = 2.5$. The extended region appears to cross the noninteracting line for lower disorder. However, the method is unable to produce meaningful results in this region.

The results in Fig. 9 contain many more points than in previous work and refer to significantly larger samples.\textsuperscript{7,14,19,22,23} It should be noted in particular that the limit of the delocalized regime around $W = 2.5$ is a factor of 2 higher than predicted by Schmitteckert\textit{ et al.} but lower than in earlier work.\textsuperscript{19}
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