A Renormalization Group Approach for Highly Anisotropic Fermion systems

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I apply a two-step density-matrix renormalization group method to the anisotropic two-dimensional tight-binding model. This study, which is a prelude to the study of models of quasi-one dimensional materials, shows the potential power of this approach for anisotropic fermionic models. I find a ground-state energy which agrees with the exact value up to four digits for systems as large as $24 \times 25$. This open new opportunities for simulations of fermions in two dimensions.

Quasi-one dimensional organic \cite{1} and inorganic \cite{2} materials have been the object of an important theoretical interest for the last three decades. The essential features of their phase diagram may be captured by the simple anisotropic Hubbard model (AHM),

$$
H = -t_\parallel \sum_{i,l,\sigma} (c_{i,l,\sigma}^\dagger c_{i+1,l,\sigma} + h.c.)
- t_\perp \sum_{i,l,\sigma} (c_{i,l,\sigma}^\dagger c_{i,l+1,\sigma} + h.c.)
+ U \sum_{i,l} n_{i,l,\uparrow} n_{i,l,\downarrow} + \mu \sum_{i,l,\sigma} n_{i,l,\sigma}.
$$

(1)

or a more general Hubbard-like model including longer range Coulomb interactions. For these highly anisotropic materials, $t_\perp \ll t_\parallel$. Over the years, the AHM has remained a formidable challenge to condensed-matter theorists. Some important insights on this model or its low energy version, the g-ology model, have been obtained through the work of Bourbonnais and Caron \cite{3,4} and others. They used a perturbative renormalization group approach to analyze the crossover from 1D to 2D at low temperatures. More recently, Biermann et al. \cite{5} applied the chain dynamical mean-field approach to study the crossover from Luttinger liquid to Fermi liquid in this model. Despite this important progress, crucial information such as the ground-state phase diagram, or most notably, whether the AHM displays superconductivity, are still unknown. So far it has remained beyond the reach of numerical methods such as the exact diagonalization (ED) or the quantum Monte Carlo (QMC) methods. ED cannot exceed lattices of about $4 \times 5$. It is likely to remain so for many years unless there is a breakthrough in quantum computations. The QMC method is plagued by the minus sign problem and will not be helpful at low temperatures. The small value of $t_\perp$ implies that, in order to see the 2D behavior, it will be necessary to reach lower temperatures than those usually studied for the isotropic 2D Hubbard model. Hence, even in the absence of the minus sign problem, in order to work in this low temperature regime, the QMC algorithm requires special stabilization schemes which lead to prohibitive cpu time.

I have shown in Ref.\cite{7} that this class of anisotropic models may be studied using a two-step density-matrix renormalization group (TSDMRG) method. The TSDMRG method is a perturbative approach in which the standard 1D DMRG is applied twice. In the first step, the usual 1D DMRG method \cite{9} is applied to find a set of low lying eigenvalues $\epsilon_n$ and eigenfunctions $|\phi_n\rangle$ of a single chain. In the second step, the 2D Hamiltonian is then projected onto the basis constructed from the tensor product of the $|\phi_n\rangle$'s. This projection yields an effective one-dimensional Hamiltonian for the 2D lattice,

$$
\tilde{H} \approx \sum_{[n]} E_{[n]} |\Phi_{[n]}\rangle \langle \Phi_{[n]}| - t_\perp \sum_{l,\sigma} (\tilde{c}_{l,\uparrow}^\dagger \tilde{c}_{l+1,\uparrow} + h.c.)(2)
$$

where $E_{[n]}$ is the sum of eigenvalues of the different chains, $E_{[n]} = \sum \epsilon_m$; $|\Phi_{[n]}\rangle$ are the corresponding eigenstates, $|\Phi_{[n]}\rangle = |\phi_{n_1}\rangle|\phi_{n_2}\rangle...|\phi_{n_L}\rangle$; $\tilde{c}_{l,\sigma}^\dagger$ and $\tilde{c}_{l,\sigma}$ are the renormalized matrix elements in the single chain basis. They are given by

$$
\tilde{c}_{l,\uparrow}^{\dagger} n_{i,l,\uparrow} m_{l,\uparrow} = (-1)^{n_{i,l}} \langle \phi_m | \tilde{c}_{l,\uparrow}^\dagger | \phi_{m_1}\rangle, \\
\tilde{c}_{l,\uparrow}^{\dagger} n_{i,l,\uparrow} m_{l,\uparrow} = (-1)^{n_{i,l}} \langle \phi_{m_1} | \tilde{c}_{l,\uparrow} | \phi_m\rangle,
$$

(3)

(4)

where $n_{i,l}$ represents the total number of fermions from sites $1$ to $i-1$. For each chain, operators for all the sites are stored in a single matrix

$$
\tilde{c}_{l,\uparrow} = (\tilde{c}_{1,\uparrow}^{\dagger}, ..., \tilde{c}_{L,\uparrow}^{\dagger}), \\
\tilde{c}_{l,\uparrow} = (\tilde{c}_{1,\uparrow}, ..., \tilde{c}_{L,\uparrow}).
$$

(5)

(6)

Since the in-chain degrees of freedom have been integrated out, the interchain couplings are between the block matrix operators in Eq. \cite{10} which depend only on the chain index $l$. In this matrix notation, the effective Hamiltonian is one-dimensional and it is also studied by the DMRG method. The only difference compare to a normal 1D situation is that the local operators are now $m_{S2} \times m_{S2}$ matrices, where $m_{S2}$ is the number of states kept during the second step.

The two-step method has previously been applied to anisotropic two-dimensional Heisenberg models. In
Ref.\cite{8}, it was applied to the $t-J$ model but due to the absence of an exact result in certain limits, it was tested against ED results on small ladders only. A systematic analysis of its performance on a fermionic model on 2D lattices of various size has not been done. In this letter, as a prelude to the study of the AHM, I will apply the TSDMRG to the anisotropic tight-binding model on a 2D lattice, i.e., The AHM with $U = 0$. I perform a comparison with the exact result of the tight-binding model.

I was able to obtain agreement for the ground-state energies on the order of $10^{-4}$ for lattices of up to $24 \times 25$. I then discuss how these calculations may extend to the interacting case.

The tight-binding Hamiltonian is diagonal in the momentum space, the single particle energies are,

$$\epsilon_k = -2t_\parallel \cos k_x - 2t_\perp \cos k_y - \mu,$$

with $k = (k_x, k_y), k_x = n_x \pi / (L_x + 1)$ and $k_y = n_y \pi / (L_y + 1)$ for open boundary conditions (OBC); $L_x, L_y$ are respectively the linear dimensions of the lattice in the parallel and transverse directions. The ground-state energy of an $N$ electron system is obtained by filling the lowest states up to the Fermi level, $E_0(N) = \sum_{k<k_F} \epsilon_k$. However in real space, this problem is not trivial and it constitutes, for any real space method such as the TSDMRG, a test having the same level of difficulty as the case with $U \neq 0$. This is because the term involving $U$ is diagonal in real space and the challenge of diagonalizing the AHM arises from the hopping term.

I will study the tight-binding model at quarter filling, $N/L_xL_y = 1/2$, the nominal density of the organic conductors known as the Bechgaard salts. Systems of up to $L_x \times L_y = (L+1) = 24 \times 25$ will be studied. During the first step, I keep enough states ($ms_1$ is a few hundred) so that the truncation error $\rho_1$ is less than $10^{-6}$. I target the lowest state in each charge-spin sectors $N_x \pm 2, N_x \pm 1, N_x$ and $S_2 \pm 1, S_2 \pm 2, N_x$ is the number of electrons within the chain. It is fixed such that $N_x/L_x = 1/2$. There is a total of 22 charge-spin states targeted at each iteration.

For the tight-binding model, the chains remain disconnected if $t_\perp < \epsilon_0(N_x + 1) - \epsilon_0(N_x)$ or $t_\perp < \epsilon_0(N_x) - \epsilon_0(N_x - 1)$, where $N_x$ is the number of electrons on single chain. In order to observe transverse motion, it is necessary that at least $t_\perp \gtrsim \epsilon_0(N_x + 1) - \epsilon_0(N_x)$ and $t_\perp \gtrsim \epsilon_0(N_x) - \epsilon_0(N_x - 1)$. These two conditions are satisfied only if $\mu$ is appropriately chosen. The values listed in Table I corresponds to $\mu = (\epsilon_0(N_x + 1) - \epsilon_0(N_x - 1))/2$. This threshold varies with $L$. I give in Table I the values of $t_\perp$ chosen for different lattice sizes. In principle, for the TSDMRG to be accurate, it is necessary that $\Delta \epsilon = \epsilon_n - \epsilon_0$, where $\epsilon_n$ is the cut-off, be such that $\Delta \epsilon/t_\perp \gg 1$. But in practice, I find that I can achieve accuracy up to the fourth digit even if $\Delta \epsilon/t_\perp \approx 5$ using the finite system method. Five sweeps were necessary to reach convergence. Note that this conclusion is somewhat different from my earlier estimate of $\Delta \epsilon/t_\perp \approx 10$ for spin systems \cite{8}. This is because in Ref.(\cite{8}), I used the infinite system method during the second step.

The ultimate success of the TSDMRG depends on the density of the low-lying states in the 1D model. For fixed $ms_2$ and $L$, it is, for instance, easier to reach larger $\Delta \epsilon/J_\perp$ in the anisotropic spin one-half Heisenberg model, studied in Ref.\cite{8}, than $\Delta \epsilon/t_\perp$ for the tight-binding model as shown in Fig. For $L = 16, ms_2 = 96$, and $J_\perp = t_\perp = 0.15$, I find that $\Delta \epsilon/J_\perp \approx 10$, while $\Delta \epsilon/t_\perp \approx 5$. Hence, the TSDMRG method will be more accurate for a spin model than for the tight-binding model. Using the infinite system method during the second step on the anisotropic Heisenberg model with $J_\perp = 0.1$, I can now reach an agreement of about $10^{-6}$ with the stochastic QMC method.

Two possible sources of error can contribute to reduce the accuracy in the TSDMRG with respect to the conventional DMRG. They are the truncation of the superblock from $4 \times ms_1$ states to only $ms_2$ states and the use of three blocks instead of four during the second step. In Table II I analyze the impact of the reduction of the number of states to $ms_2$ for three-leg ladders. The choice of three-leg ladders is motivated by the fact that at this point, the TSDMRG is equivalent to the exact diagonalization of three reduced superblocks. It can be seen that as far as $t_\perp \gtrsim \epsilon_0(N_x + 1) - \epsilon_0(N_x)$ and $t_\perp \gtrsim \epsilon_0(N_x) - \epsilon_0(N_x - 1)$, the TSDMRG at this point is as accurate as the 1D DMRG.

![Graph showing low-lying states of the 1D tight-binding model](image)

**Fig. 1:** Low-lying states of the 1D tight-binding model (full line) and of the 1D Heisenberg spin chain (dotted line) for $L = 16$ and $ms_2 = 96$.

| $L$     | $ms_2$ | $\Delta \epsilon/t_\perp$ |
|---------|--------|-----------------------------|
| $8 \times 9$ | 16 \times 17 | 24 \times 25 |
| $t_\perp$ | -0.28  | -0.15  | -0.1 |
| $\mu$    | -1.2660 | -1.3411 | -1.3657 |
| $\Delta \epsilon/t_\perp$ | 6.42  | 5.40  | 5.78  |

**Table I:** Transverse hopping and chemical potential used in the simulations for different lattice sizes
Note that the accuracy remains nearly the same irrespective of $L$ as far as the ratio $\Delta \epsilon/t_\perp$ remains nearly constant. Since $\Delta \epsilon$ decreases when $L$ increases, $t_\perp$ must be decreased in order to keep the same level of accuracy for fixed $ms_2$. In principle, following this prescription, much larger systems may be studied. $\Delta \epsilon/t_\perp$ does not have to be very large, in this case it is about 5, to obtain very good agreement with the exact result.

The second source of error is related to the fact that the effective single site during the second step is now a good agreement with the exact result. For fixed $ms_2$, in this case it is about 5, to obtain very good agreement with the exact result.

The agreement with the exact result is very good and to be described accurately themselves. A larger weight on these additional states would lead to the reduction of the accuracy for a fixed $ms_2$. In Table III, I show the improved energies when, besides the ground state, I target the lowest states of the spin sectors $S_z = -1$ and $S_z = +1$ with $N$ electrons. The weights were respectively 0.995, 0.0025, and 0.0025 for the three states. This lowers $E_{\Psi_0}(N)$ in all cases, but the gain does not appear to be spectacular. But I do not know whether this is due to my choice of perturbation of $\rho$ or whether even the algorithm with four blocks would not yield better $E_{\Psi_0}(N)$. If the lowest sectors with $N + 1$ and $N - 1$ electrons which have $S_z = \pm 0.5$ are projected instead, I find that the results are similar to those with $S_z = \pm 1$ sectors, there are possibly many ways to add the missing states. A more systematic approach to this problem has recently been suggested [11]. It is based on using a local perturbation to build a correction to the density matrix from the site at the edge of the system. Here, such a perturbation would be $\Delta \rho = \alpha c_1^\dagger c_1$, where $\alpha$ is a constant, $\alpha \approx 10^{-3} - 10^{-2}$, and $c_1^\dagger$, $c_1$ are the creation and annihilation operators of the chain at the edge of the system. This type of perturbation resulted in an accuracy gain of more than an order of magnitude in the case of a spin chain [11]. The three block method was found to be on par with the four block method. It will be interesting to see in a future study how this type of local perturbation performs within the TSDMRG.

To conclude, as a first step to the investigation of interacting electron models, I have shown that the TSDMRG can successfully be applied to the tight-binding model. The agreement with the exact result is very good and can be improved since the computational power involved in this study was modest. The extension to the AHM with $U \neq 0$ is straightforward. There is no additional change in the algorithm since the term involving $U$ is local and thus treated during the 1D part of the TSDMRG. The role of $U$ is to reduce $\Delta \epsilon$ as shown in Fig 4. For fixed $L$ and $ms_2$, $\Delta \epsilon$ decreases linearly with increasing $U$. For

\begin{table}[h]
\centering
\begin{tabular}{|c|c|c|c|}
\hline
$ms_2$ & $8 \times 3$ & $16 \times 3$ & $24 \times 3$ \\
\hline
64 & -0.241524 & -0.211929 & 0.204040 \\
100 & -0.24819 & -0.21414 & 0.20509 \\
120 & -0.24832 & -0.21419 & 0.20519 \\
Exact & -0.24857 & -0.21432 & 0.20519 \\
\hline
\end{tabular}
\caption{Ground-state energies for three-leg ladders; a single state was targeted in the second step.}
\end{table}

\begin{table}[h]
\centering
\begin{tabular}{|c|c|c|c|}
\hline
$ms_2$ & $8 \times 9$ & $16 \times 17$ & $24 \times 25$ \\
\hline
64 & -0.24761 & -0.21401 & 0.20554 \\
100 & -0.24819 & -0.21414 & 0.20509 \\
120 & -0.24832 & -0.21419 & 0.20519 \\
Exact & -0.24857 & -0.21432 & 0.20519 \\
\hline
\end{tabular}
\caption{Ground-state energies for different lattice sizes; three states were targeted in the second step: the ground state itself and the lowest states of $S_z = 0$ and $S_z = 1$ sectors.}
\end{table}
L = 16 and $m s_2 = 128$, I anticipate that for $U \lesssim 3$ the interacting system results will be on the same level or better than those with $m s_2 = 100$ for the same value of $L$.

I wish to thank A.M.-S. Tremblay for very helpful discussions. I thank K.L. Graham for reading the manuscript. This work was supported by the NSF Grant No. DMR-0426775.

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