Density Matrix Renormalization Group Study of
One-Dimensional Acoustic Phonons.

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Abstract

We study the application of the density matrix renormalization group (DMRG) to systems with one-dimensional acoustic phonons. We show how the use of a local oscillator basis circumvents the difficulties with the long-range interactions generated in real space using the normal phonon basis. When applied to a harmonic atomic chain, we find excellent agreement with the exact solution even when using a modest number of oscillator and block states (a few times ten). We discuss the use of this algorithm in more complex cases and point out its value when other techniques are deficient.
In a previous paper [1], we have studied how the real-space density matrix renormalization group (DMRG) [2] could be applied to dispersionless phonons in the ground state of magnetic or fermion chains. We showed that the unavoidable truncation of the local oscillator space proved manageable for a Peierls or spin-Peierls deformation. Acceptable numerical accuracy could be obtained by properly selecting the dimension of the oscillator space as a function of the amplitude of the lattice deformation (the Peierls gap).

The true Peierls, spin-Peierls, and superconductivity problems, or more generally the electron-phonon problem, however, involve acoustic phonons having dispersion. Are the hydrodynamic modes problematic? Let us look at other numerical approaches and see how they deal with phonons. Although the dispersion has not created any difficulty in exact diagonalization calculations on a one-dimensional (1D) lattice [1], most efforts with electron-phonon systems have used dispersionless phonons [2] or have focused on a single acoustic mode related to an order parameter [2]. The reason was to keep the dimension of the quantum space tractable. The chain or cluster size being rather small (of order 10 sites), however, there is little hope of doing numerical justice to the hydrodynamic modes.

The quantum Monte Carlo method (QMC) [3] has apparently done very well with acoustic phonons and the hydrodynamic modes. The QMC does have sign problems, however, with the electronic part in frustrated systems and with some magnetic impurity problems [4]. There is no problem with phonons, of course, in a momentum space formulation of the DMRG [1]. The treatment of local interactions (Hubbard interaction, exchange interaction, electron-phonon interaction...) is, however, more complex and computationally exacting in momentum space.

The DMRG has the capability of reaching chain lengths in the hundreds, is free of the sign problem of the QMC, and is ideally suited to short-range interactions. The situation with the hydrodynamic modes is potentially troublesome, however. The long-range displacement-displacement autocorrelation function \( \langle (u_\ell - u_{\ell'})^2 \rangle \) in an infinite chain increases logarithmically with the distance \( R_{\ell\ell'} \) between the static (classical) atomic equilibrium positions. The same is true of the displacement amplitude squared \( \langle (u_\ell)^2 \rangle \) at the center of a finite chain.
with closed boundary conditions (fixed ends) which grows logarithmically with the number \( N_a \) of atoms in the chain. As a consequence, the amplitude of the atomic displacements can grow without bounds as the chain length increases in the DMRG procedure. In other words, there is no fixed point for the infinite-chain DMRG algorithm. It is forever fleeting as the chain grows. There is also another constraint on the form the Hamiltonian should have in the DMRG. The procedure takes place in real space and, ideally, the Hamiltonian should be reducible to a form involving only short-range coupling terms between the central site(s) and the two adjacent blocks. Otherwise, the numerical accuracy and memory expenditures - for the storage of the block variables coupling to the central site(s) - suffer greatly. It so turns out, as we shall see below, that using the normal phonon coordinates, defined in momentum space, leads to long-range couplings in real space and thus to potential difficulties for the DMRG.

It is the purpose of this paper to study the constraints imposed by these considerations on the DMRG treatment of the ground state of a chain bearing acoustic phonons. We have chosen to focus specifically on the phonons leaving aside any electronic or spin counterpart. There are well documented applications of the DMRG to spin \[3\] \[10\] \[11\], electron \[12\] or mixed \[13\] systems. As such, the atomic chain problem is more a testing ground for the DMRG than a physical problem since its excitations and thermodynamics have exact solutions.

We shall study finite chains having \( N_a \) atoms and closed boundary conditions. Keeping the end atoms at fixed positions eliminates the troublesome \( q = 0 \) mode which, for periodic or open boundary conditions, corresponds to uniform displacements (and unbounded \( \langle (u_\ell)^2 \rangle \)). We shall assume the usual harmonic Hamiltonian

\[
H = \sum_\ell \frac{p_\ell^2}{2m} + \frac{1}{2}K \sum_\ell (u_\ell - u_{\ell+1})^2
\]

and the boundary conditions \( u_1 = u_{N_s} = 0 \). The solutions are of course well known in terms of the annihilation \( d_q \) and creation \( d_q^\dagger \) operators for the normal modes of momentum \( q = n\pi N^{-1}_\text{mod}, \ 1 \leq n \leq N_{\text{mod}}, \) where \( N_{\text{mod}} = (N_a - 2) \) is the number of normal modes. One
has simply

\[ H = \sum_q \hbar \omega_q (d_q^\dagger d_q + \frac{1}{2}) , \]

where the eigenfrequency is \( \omega_q = 2\sqrt{K/m} |\sin(q/2)| \). Here and throughout, we have put the static equilibrium interatomic distance equal to one.

The need for writing the Hamiltonian in real space stems from the real space algorithm used in the DMRG. In the case of our Eq. 2, one could try to exploit the operators \( d_\ell = N_{\text{mod}}^{-\frac{1}{2}} \sum_q \exp(iq\ell) d_q \) on the perhaps natural reflex of using the diagonal phonon annihilation operators. Unfortunately, the Hamiltonian in real space then has the form

\[ H = \sum_{\ell, \ell'} F(\ell' - \ell) d_{\ell'}^\dagger d_\ell + \frac{1}{2} \sum_q \hbar \omega_q , \]

\[ F(x) = N_{\text{mod}}^{-1} \sum_q \hbar \omega_q \exp(ix) . \]

The \( F(x) \) function is slowly decreasing, varying as \( x^{-2} \), at long distances. Consequently, the block operators \( \mathcal{O}_{\ell'\ell} = F(\ell' - \ell) d_\ell \) are relevant for all sites \( \ell' \) in the blocks. The storage requirements are large. The number of stored elements is of order \( N_{bs} M_b^2 \) at each step \( s \), for the infinite-chain algorithm, where \( N_{bs} \) and \( M_b \) are the number of atoms and the number of selected states in each block, respectively. It is huge, of order \( \sum_s N_s M_b^2 \), for the finite-chain algorithm, the sum covering all steps \( s \) of the procedure. The numerical accuracy would greatly suffer.

There is a second problem, for the infinite-chain algorithm, related to the quantization of the phonon momentum \( q \). Its values depend on the chain length \( N_a \) and thus change from step to step. Consequently, so does the amplitude \( F(x) \) of the coupling terms. This is rather annoying. This problem can of course be circumvented by using the finite-chain algorithm as one can use the \( q \) values of the chosen chain length.

The way around these problems is to use another basis set of quantum oscillators. Let us use instead the local oscillators (as in [4]) that are solutions of

\[ H_o = \sum_\ell \frac{p_\ell^2}{2m} + K \sum_\ell (u_\ell)^2 = \sum_\ell \hbar \omega_o (b_\ell^\dagger b_\ell + \frac{1}{2}) , \]
where $\omega_o = \sqrt{2K/m}$, $u_\ell = (\frac{\hbar}{2m\omega_o})^{\frac{1}{2}}(b_\ell^\dagger + b_\ell)$. With this construction, one can write
\[ H = H_o + H_c \tag{5} \]
where
\[ H_c = -K \sum_\ell u_\ell u_{\ell+1} = -\frac{\hbar \omega_o}{4} \sum_\ell (b_\ell^\dagger + b_\ell)(b_{\ell+1}^\dagger + b_{\ell+1}) . \]
This expression for $H$ is exact. The coupling terms $H_c$ are now, however, short ranged and independent of the chain length. This last formulation is thus highly preferable for use with the DMRG even though the local oscillators are not diagonal. As a matter of fact, the connection between the $b_\ell$ and the $d_q$ is not trivial:
\[ b_\ell = N_{mod}^{-\frac{1}{2}} \sum_q \left[ (\frac{\omega_o}{2\omega_q})^{\frac{1}{2}} + (\frac{\omega_q}{2\omega_o})^{\frac{1}{2}} \right] \sin(q\ell)d_q \]
\[ \quad + \left[ (\frac{\omega_o}{2\omega_q})^{\frac{1}{2}} - (\frac{\omega_q}{2\omega_o})^{\frac{1}{2}} \right] \sin(q\ell)d_q^\dagger . \tag{6} \]
This is a canonical transformation. We shall now study the implementation of Eq. 5.

As mentioned in the Introduction, the central atom(s) oscillator space must be truncated at a dimension sufficient to properly represent the vibrational motion of the atoms. Regardless of the algorithm used, one must begin by using the infinite-chain algorithm which is plagued by the absence of any fixed point. Indeed, the vibrational amplitude of the central atom was already mentioned to be logarithmically increasing at each step:
\[ \langle (u_\ell)^2 \rangle = N_{mod}^{-1} \sum_q \left( \frac{\hbar}{m\omega_q} \right) (\sin(q\ell))^2 \propto \ln(N_a) . \tag{7} \]
This last quantity is a measure of the average occupation number $\langle n_\ell \rangle$ of the local oscillator. It is then a prerequisite that the dimension $M_\nu$ of the local oscillator space be sufficient to cover the requirements of Eq. 7, that is $M_\nu \gg \langle n_\ell \rangle$. Our previous experience [1] has revealed that this dimension should be of order ten. We have thus used only one central atom (site) in order to keep the computation time and storage requirements within acceptable values. We
have monitored the occupation probability \( P_s(n) \) of each oscillator state \( |n\rangle = (n!)^{-\frac{1}{2}} (b_{\ell}^{\dagger})^{n} |0\rangle \), \( 0 \leq n \leq M_{\nu} \), of the central atom for each step \( s \) of the infinite-chain algorithm for \( N_a \) up to 49 atoms. We find that \( P_s(n) \approx 0.35 \exp(-n/\alpha_s) \), \( \alpha_s \approx .33 + .18 \ln(N_a - 3) \), fits the data quite well for most occupations, except for the first and last ones \( n = 0, M_\nu - 1 \). Notice the logarithmic dependence for \( \alpha_s \) which weighs the average and the standard deviation for the local oscillator occupation. Having this information, one can estimate a minimal relative error on the oscillator space statistics \( \delta P_s \approx P_s(M_\nu - 1) \) at each step resulting from using a finite dimensional oscillator space for the central atom. This error is propagative and thus, the total minimum numerical error of a sweep should be expected to be of order \( \delta P \approx \sum_s P_s(M_\nu) \). One can thus use this criterion to determine the minimal requirement on \( M_\nu \) for the situation at hand.

As the finite-chain method leads to the greatest precision [3], let us first look at some results using this algorithm. Table I lists a few runs for a 25 atom chain. We have found that two sweeps are sufficient in all situations. Further sweeping changes little to the numerical values. Table I shows the various parameters used in each run: the oscillator space dimension \( M_\nu \), the number of block states kept \( M_b \), the number of target states \( M_t \), and the estimated minimal error \( \delta P \) arising from the truncated oscillator space. We have calculated the numerical error on the ground state correlation energy \( \delta E_{corr} = (E_{corr}^{DMRG} - E_{corr}^{o})/E_{corr}^{o} \), where \( E_{corr} = E_{gs} - \frac{1}{2} N_{mod} \hbar \omega_o \) and \( E_{gs} \) is the ground state energy. The superscripts "DMRG" and "o" refer to the computational and the exact values, respectively. Note that \( E_{gs}^{o} = \frac{1}{2} \sum_q \hbar \omega_q \). This correlation energy is more significant than \( E_{gs} \) since the zero point energy of the local oscillators is not a numerically meaningful quantity. We have also calculated the error on the correlation function between the central atom and its first neighbor \( \delta C = |\langle (u_{\ell} - u_{\ell-1})^2 \rangle_{DMRG} - \langle (u_{\ell} - u_{\ell-1})^2 \rangle_{o}| / \langle (u_{\ell} - u_{\ell-1})^2 \rangle_{o} \), the one on the oscillation amplitude square of the central atom \( \delta U = |\langle (u_{\ell})^2 \rangle_{DMRG} - \langle (u_{\ell})^2 \rangle_{o}| / \langle (u_{\ell})^2 \rangle_{o} \), and the error on the average oscillator occupancy of the central atom \( \delta n = |\langle n \rangle_{o} - \langle n \rangle_{DMRG}| / \langle n \rangle_{o} \). \( \langle n \rangle_{o} = \langle b_{\ell}^{\dagger} b_{\ell} \rangle_{o} \), while \( u_{\ell} \) and \( b_{\ell} \) are defined in Eq. 4 and 6 respectively. The run with 11
oscillator states and $M_b = 10$ shows $\delta E_{\text{corr}}$ to be roughly of the same size as $\delta P$. Increasing $M_\nu$ does not change $\delta E_{\text{corr}}$ much. A saturation level has been reached for $M_\nu \geq 11$ even though $\delta P$ keeps on decreasing. The central oscillator space is sufficiently large that enlarging it any further does little. Why is this? The reason is that important information contained in the central site is not being relayed to the next iteration step because too few block states are kept. Indeed, doubling $M_b$, as in the last run, considerably reduces the error on the ground state energy. One notices that the error on the nearest-neighbor correlation is of the same order as $\delta E_{\text{corr}}$. The errors $\delta U$ and $\delta n$, however, are of the same order but much larger than $\delta E_{\text{corr}}$. This is systematically found in all our simulations. The reason is that these quantities sample the local oscillator excitations to a much larger degree than the other quantities. The accuracy on excitation energies is less than on the energy in the DMRG. Similar findings, shown in Table I, were obtained for 49 and 99 atom chains.

In Table I, we used the infinite-chain algorithm to look at the effect of increasing the number of target states. We see that the accuracy gets better when using a few target states and worsens when using too many. This is quite typical of the DMRG [11]. Using four target states transfers better information, through the projection procedure, to the block states and improves $\delta n$ considerably. Using too many target states dilutes the relevant information with irrelevant one. The runs with 30 block states show that the infinite-chain algorithm with four target states can perform as well as the finite-chain one (compare to the last entry in Table I) although the latter has just a single target state and a smaller number of block states. One then has to weigh the numerical expenditure of having more states as compared to doing two sweeps. This result is most important as it shows how to make a proper use the infinite-chain algorithm.

We have shown that expressing the Hamiltonian in terms of local oscillators leads to a short-range coupling between blocks and central atom(s). This is a nice property to have when implementing the DMRG procedure. We have observed that the numerical error introduced by the truncation of the local oscillator space can be satisfactorily controlled by ab-initio selection of the size of the oscillator space for the problem at hand. This applies to
any chain-length envisaged. We have found that the number of block states $M_b$ to be used is quite critical to the accuracy. As a rule of thumb, one should keep at least something like 2 times the dimension of the local oscillator space $M_ν$. More important though, we have shown that the infinite chain algorithm can be used in spite of the anticipated limitations with regard to the lack of a fixed point and the logarithmic dependence of the atomic motion as a function of chain length.

We have also found the usual DMRG truncation error $δE_{\text{trunc}}$ is useless as an error indicator. We monitored it and observed it to be much smaller than the error on the correlation energy $δE_{\text{corr}}$ or even $δP$. This is rather puzzling since, as seen in the previous section, important errors stem from the quality of the projection of the target states onto the block states. The reason has to do with the limited information contained in the ground state of the super block with regard to the central site. The central site of the super block is an inversion symmetry center whereas it no longer is so at the end of the new block. The symmetry breaking information that is required for a proper description of the last site of the new block is thus contained in block states that have little statistical weight in the density matrix.

The Hamiltonian we have studied is of an academic nature. By choosing the local oscillator basis, we knowingly sacrificed its phonon conservation law in order to obtain a form that is in harmony with the DMRG procedure. Our study does, however, provide a necessary stepping stone for problems that do not conserve the number of phonons. These are the more physical situations like the Peierls or spin-Peierls chains or, quite generally, the electron-phonon problem in one dimension. The computational expenditure required for phonons is rather modest and would presumably remain so in electron-phonon or spin-phonon problems with a gap as in [1].

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TABLES

TABLE I. Finite-chain algorithm for 25 atoms. The parameters are: the oscillator space dimension $M_ν$, the number of block states $M_b$, the number of target states $M_t$, the estimated minimal error on the oscillator statistics $δP$, the numerical error on the ground state correlation energy $δE_{corr}$, the one on the correlation function between the central atom and its first neighbor $δC$, the one on the oscillation amplitude squared of the central atom $δU$, and the error on the average oscillator occupancy of the central atom $δn$.

| $M_ν$ | $M_b$ | $M_t$ | $δP$ | $δE_{corr}$ | $δC$ | $δU$ | $δn$ |
|-------|-------|-------|------|-------------|------|------|------|
| 11    | 10    | 1     | $10^{-5}$ | $1.9 \times 10^{-5}$ |       |      | 0.013 |
| 15    | 10    | 1     | $10^{-7}$ | $1.1 \times 10^{-5}$ | $8.4 \times 10^{-5}$ | 0.0032 | 0.006 |
| 20    | 10    | 1     | $4 \times 10^{-10}$ | $1.1 \times 10^{-5}$ |       |      | 0.0059 |
| 15    | 20    | 1     | $10^{-7}$ | $2.8 \times 10^{-6}$ | $2.6 \times 10^{-6}$ | $1.7 \times 10^{-4}$ | $3.6 \times 10^{-4}$ |

TABLE II. Finite-chain algorithm for chains of $N_a$=49 and 99 atoms. The parameters are defined in Table I.

| $M_ν$ | $M_b$ | $M_t$ | $N_a$ | $δP$ | $δE_{corr}$ | $δC$ | $δU$ | $δn$ |
|-------|-------|-------|-------|------|-------------|------|------|------|
| 15    | 10    | 1     | 49    | $3 \times 10^{-6}$ | $4.4 \times 10^{-4}$ | $2.1 \times 10^{-4}$ | 0.026 | 0.05  |
| 15    | 20    | 1     | 49    | $3 \times 10^{-6}$ | $2.5 \times 10^{-5}$ | $1.6 \times 10^{-5}$ | 0.0032 | 0.006 |
| 20    | 20    | 1     | 49    | $10^{-8}$ | $1.3 \times 10^{-5}$ | $1.2 \times 10^{-5}$ | 0.0014 | 0.0026 |
| 20    | 30    | 1     | 49    | $10^{-8}$ | $2.1 \times 10^{-6}$ | $8.8 \times 10^{-7}$ | $2.2 \times 10^{-4}$ | $4.0 \times 10^{-4}$ |
| 15    | 20    | 1     | 99    | $3 \times 10^{-5}$ | $9.8 \times 10^{-5}$ | $4.7 \times 10^{-5}$ | 0.028 | 0.045 |
| 20    | 30    | 1     | 99    | $3 \times 10^{-7}$ | $1.1 \times 10^{-5}$ | $3.2 \times 10^{-6}$ | 0.0038 | 0.0063 |
TABLE III. Infinite chain algorithm for 25 atoms. The parameters are defined in Table I.

| $M_\nu$ | $M_b$ | $M_t$ | $\delta E_{corr}$ | $\delta n$ |
|---------|-------|-------|-------------------|-----------|
| 15      | 20    | 1     | $3.7 \times 10^{-4}$ | 0.0035    |
| 15      | 20    | 4     | $2.8 \times 10^{-4}$ | 0.0015    |
| 15      | 20    | 7     | $1.7 \times 10^{-3}$ | 0.0085    |
| 15      | 30    | 4     | $2.6 \times 10^{-5}$ | $3.5 \times 10^{-4}$ |
| 15      | 30    | 1     | $1.5 \times 10^{-4}$ | 0.00145   |