Recursive computation of Green’s functions for interacting particles in disordered lattices and binary trees

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Abstract. In this article, the method of computing Greens functions recursively for interacting particles has been extended to square lattices and binary trees. The method allows for performing calculations for large lattices. Approximations, which make the method more efficient while maintaining accuracy are described for computations of dynamics and correlations of interacting particles in disordered systems. Direct informations related to spectral weights for different initial preparations of interacting particles in real space can be obtained using this method for larger system sizes with less finite size effects.

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1. Introduction

Knowing the behavior of interacting particles is one of the main goals of condensed matter physics. Calculation of two particle Green’s function is considered to be most fundamental tool in understanding such behaviors [1] [2]. The two-particle correlations are known to play an important role in properties of many lattice systems [3] [4] [5] [6][7]. However, these calculations become extremely difficult for larger system sizes. Most often the approach that is taken is that of full diagonalization. However, the matrices involved in such diagonalizations are sparse and an efficient recursive
method can be developed using this sparsity for certain systems such as particles in lattices with nearest neighbor hopping. The tight-binding model Hamiltonians can be readily solved by continued fraction method, which was applied by Haydock et al [8] and Morita [9] as early as in the 1970s for calculation of density of states in ideal 3D lattices of various kinds. Recently, an efficient formulation in momentum space for ideal lattices was developed to calculate few-particle Green’s functions, which also elucidated the effect of the interaction on few-particle bound complexes [10 11 12].

In recent times, phenomenal advances has been achieved in experiments with ultracold atoms [13 14] and trapped ions [15 16 17] to observe and control the dynamics of interacting particles. Such experiments can not only make measurements on single site resolution [21 22] but also count for joint site occupations [23 24]. Experiments on rotational excitations of trapped dipolar molecules [25 26 27 28 29 30] has also been achieved. Experiments on photonic systems based on waveguide lattices has also been performed [18 19 20]. The particles in these systems approximately undergo unitary dynamics within the consideration of timescale of the experiments. Green’s functions does provide a direct approach to calculate such unitary dynamics of interacting particles. Such experiments [31 32 18 19 20] not only provides understanding on effects of interactions on two-particle correlations but also verifies theoretical predictions.

A method, where such two-particle Green’s functions can be efficiently calculated in both ideal and disordered systems has been developed [33] for 1D systems. In this article, it is extended to 2D systems and shown to be exactly mappable to some arbitrary graphs (e.g. binary trees). The method allows for calculations of two-particle Green’s functions for fairly large lattices. For disordered lattices, the calculations can be made more efficient with approximations that reduce the difficulty of calculations significantly without significant errors. These approximations are described in later sections explaining their applicability.

The algorithm is explained in the next section. Few calculations of correlation dynamics and properties such as the density of states and the spectral weight of the two interacting particles in 1D and 2D lattices and in binary trees are described in the result section.
2. Algorithm

The Green’s function for some hamiltonian $H$ is defined as following:

$$G(\omega) = \frac{1}{\omega - H}$$  \hspace{1cm} (1)

where $\omega = E + \eta$ is a complex number with $\eta$ a very small positive real number and $G(m, n, \omega) = \langle mn | G(\omega) | m'n' \rangle$ is a time-independent propagator from two particles occupying sites $m'$, $n'$ to sites $m$, $n$ in the 1D lattice. We omit the indices $m'$, $n'$ wherever unnecessary for brevity from now on.

For a hamiltonian of the form of Eq. 2, where $\epsilon_m$ is the onsite energy, $t_{mn}$ is the hopping element moving the particle from site $m$ to site $n$ and $v_{mn}$ is the interaction between particles at sites $m$ and $n$,

$$H = \sum_m \epsilon_m a_m^\dagger a_m + \sum_{\langle mn \rangle} t_{mn} a_m^\dagger a_n + \sum_{\langle mn \rangle} V_{mn} a_m^\dagger a_n a_m, \hspace{1cm} (2)$$

the following type of recurrence relations will emerge. Here, the vectors $\langle mn |$ from left and $| m'n' \rangle$ from right to the identity $(\omega - H)G(\omega) = 1$ from Eq. 1 have been multiplied to find the relations for functions like $G(m, n, \omega)$ sorted on the left hand side of Eq. 3 and their related Green’s functions on the right hand side.

$$(\omega - \epsilon_{m-1} - \epsilon_{n+1} - V_{m-1n+1})G(m-1, n+1, \omega) = \delta_{m-1,m'}\delta_{n+1,n'} + \delta_{m-1,n'}\delta_{n+1,m'}$$
$$- t_{m-2,m-1}G(m-2, n+1, \omega)$$
$$- t_{m,m-1}G(m, n+1, \omega)$$
$$- t_{n,n+1}G(m-1, n, \omega)$$
$$- t_{n+2,n}G(m-1, m+2, \omega)$$

$$(\omega - \epsilon_{m} - \epsilon_{n} - V_{mn})G(m, n, \omega) = \delta_{m,m'}\delta_{n,n'} + \delta_{m,n'}\delta_{n,m'}$$
$$- t_{m-1,m}G(m-1, n, \omega)$$
$$- t_{m+1,m}G(m+1, n, \omega)$$
$$- t_{n-1,n}G(m, n-1, \omega)$$
$$- t_{n+1,n}G(m, n+1, \omega)$$

$$(\omega - \epsilon_{m+1} - \epsilon_{n-1} - V_{m+1n-1})G(m+1, n-1, \omega) = \delta_{m+1,m'}\delta_{n-1,n'} + \delta_{m+1,n'}\delta_{n-1,m'}$$
$$- t_{m,m+1}G(m, n-1, \omega)$$
Here, only nearest neighbor hopping and interaction is considered. Once all $G(m, n, \omega)$ are found, the dynamics can be easily computed by the Fourier transformation of the Green’s function amplitudes from the energy domain to the time domain

$$G(m, n, t) = \sum_{\omega} e^{-i\omega t} G(m, n, E + \eta). \quad (4)$$

The spectral weight for any initial state of the two particles at sites $m'$ and $n'$, can be computed from a single Green’s element

$$A(m', n', E) = \frac{-1}{\pi} \text{Im}[G(m', n', E + i\eta)]. \quad (5)$$

The density of states (DOS) of the lattice systems up to a scaling factor can also be computed from all such single Green’s elements

$$\text{DOS}(E) = \sum_{m', n'} A(m', n', E). \quad (6)$$

If there is translational symmetry present in the system, then only a few initial states with increasing relative distance ($|m' - n'|$) might prove sufficient for convergence.

Now, the recursive functions are formulated in the form of Eq. 3 consisting of vectors in a chain. One needs to first find some good quantum numbers and group Green’s elements according to such numbers. We find $R=m+n$ for the Green’s functions of the form $G(m, n, \omega)$ in real space is such a number, as the hamiltonian does not connect functions with same $R$ directly, as can be checked from Eq. 3. We sort all such functions in a single vector $\mathcal{G}_R$, as in Eq. 7. One can also notice that $\mathcal{G}_R$ is only connected to $\mathcal{G}_{R-1}$ and $\mathcal{G}_{R+1}$ by the hamiltonian, as in the Eq. 8

$$\mathcal{G}_{R=m+n}(\omega) = \begin{pmatrix} \cdot \\ G(m-1, n+1, \omega) \\ G(m, n, \omega) \\ G(m+1, n-1, \omega) \\ \cdot \end{pmatrix} \quad (7)$$
\[ G_R = \alpha_R g_{R-1} + \beta_R g_{R+1} + C \]  

(8)

where \( C = 0 \) (or \( \neq 0 \)) when \( R \neq m' + n' \) (or = \( m' + n' = R' \)).

These vectors form a one dimensional chain in terms of their connection to only the nearest neighbor vectors and each of their elements can be solved exactly by the following prescription. This particular form also appears in many other areas of quantum physics and therefore a similar method in principle can be constructed.

On the left and right boundary of the chain, the following equations hold

\[ G_0 = \beta_0 g_1 \text{ and } G_L = \alpha_L g_{L-1}, \]  

(9)

where 0 and \( L \) are the minimum and maximum index possible for \( R \).

If we can simplify Eq. 8 as in Eq. 9 then all the calculations will become a recursion of vectors:

\[ G_R = A_R g_{R-1} \text{ and } G_R = B_R g_{R+1}, \text{ for } R \neq R'. \]  

(10)

We find \( A_0 = \beta_0 \) and \( B_L = \alpha_L \). These are our open boundary conditions. Now, substituting Eq. 10 to Eq. 8 for \( R < R' \) and \( R > R' \), we find the following equations respectively:

\[ G_R = \alpha_r g_{R-1} + \beta_r g_{R+1} \]
\[ B_R g_{R+1} = \alpha_r B_{R-1} g_R + \beta_r g_{R+1} \]
\[ B_R g_{R+1} = \alpha_r B_{R-1} B_R g_{R+2} + \beta_r g_{R+1} \]
\[ B_R = [1 - \alpha_r B_{R-1}]^{-1} \beta_r \]  

(11)

\[ G_R = \alpha_r g_{R-1} + \beta_r g_{R+1} \]
\[ A_R g_{R-1} = \alpha_r g_{R-1} + \beta_r A_{R+1} g_R \]
\[ A_R g_{R-1} = \alpha_r g_{R-1} + \beta_r A_{R+1} A_R g_{R-2} \]
\[ A_R = [1 - \beta_r A_{R+1}]^{-1} \alpha_r \]  

(12)

One can compute these \( A_R \) and \( B_R \) matrices recursively starting from Eq. 9 before one reaches \( R = R' \) from both sides of the chain. At \( R = R' \), applying \( A_{R+1} \) and \( B_{R-1} \) to Eq. 8 one finds the following:
\[ G_{R'} = \alpha R G_{R'-1} + \beta R G_{R'+1} + C, \]
\[ G_{R'} = \alpha R B_{R'-1} G_{R'} + \beta R A_{R'+1} G_{R'} + C, \]
\[ G_{R'} = [1 - \alpha R B_{R'-1} - \beta R A_{R'+1}]^{-1} C. \] (13)

Once \( G_{R'} \) is found, all other \( G_R \) can be found by Eq. (10), hence solving the problem of finding all the Green’s elements for a given \( m' \) and \( n' \) for a single \( \omega \) without diagonalization. To find all the eigenenergies, one has to scan over a range of \( \omega \) that can be used in Eq. (4) to compute dynamics. The calculations for each \( \omega \) are distinct from each other and can be parallelized. The value of \( \eta \) has to be chosen arbitrarily. This choice can be benchmarked by comparing a few sample calculations with full diagonalization.

3. Results

In this section few Green’s functions of interest are described. These are the functions which provide direct information on spectral weights, density of states, dynamics and localization parameters. For disordered systems, localization parameter as inverse participation ratio (IPR) can be calculated from many Green’s functions. However, these calculations become difficult for larger system sizes in the cases of two dimensional systems and approximations are found to be producing results without significant error while reducing the computation hurdle. This recursive algorithm is an enabler for performing computations of large system sizes. The calculations become more efficient as it splits the full matrix to multiple smaller matrices and with higher degree of parallelizations, the computations can be turned even more efficient.

Figure 1 describe calculation of \( G(m', n', \omega) \) for \( |m' - n'| = 1 \) for an ideal 1D lattice size of 500 sites. The particles were taken as hard-core bosons in ideal lattices following the tight binding hamiltonian as in Eq. (14)

\[ H = \sum_{\langle mn \rangle} t a_m^\dagger a_n + \sum_{\langle mn \rangle} V a_m^\dagger a_n a_m \] (14)

The DOS calculations performed for a smaller lattice system of 80 sites with full diagonalization are shown as a reference. The algorithm can be used to perform
Figure 1: Density of states (DOS) calculated for a 1D ideal lattice of two interacting particles from full diagonalization are plotted as dotted lines. The spectral weights for two particles initially located at adjacent sites calculated using Eq. 5 is shown in straight lines. The inset shows calculation of density of states using Eq. 6.

calculations for 1D lattices with more than thousand sites. For larger lattices the calculated Green’s functions are smooth indicative of reduced finite size effects.

For the calculations of correlation dynamics, one requires all Green’s functions for each energy point \( E \) within the band. Agreement with full diagonalization becomes better with higher number of energy points involved in calculations. Excellent agreement between results calculated using recursive algorithm with that obtained from full diagonalization is shown in Fig. 2. The effectiveness of the method can be realized even by searching less than 500 points (for each \( E \) needed in Eq. 4) within the full the energy band \((-4 \leq E \leq +4)\). Calculations with less than 50 points per unit of the band width turns out to start producing errors in the range
Figure 2: Comparison between recursive calculation using only 10(left) and 50(middle) search points per unit bandwidth with that of full diagonalization(right) for correlation dynamics of two particles in a 1D ideal lattice for $V = 1$ and at $time = 10$ (in the unit of hopping).

of a unit percentage in such calculations. The approach of first finding the most important bandwidth from the calculated spectral weight can also be adopted which minimizes the number of search points and enhances the efficiency of the computation in such calculations.

The algorithm is particularly useful for calculations of Green’s functions in systems with disorder. Figure 3 shows the imaginary part of a few randomly selected Green’s functions for a fixed initial state and final occupations at different distance (minimum number of steps between two particles) in a disordered 2D lattice. The recursive calculations match exactly with that of full diagonalization irrespective of the distance between the two particles. However, there are possibilities of numerical errors depending on the implementation of the algorithm. To calculate localization properties of disordered systems, where averaging over many realizations of disorder is required to account for robust results, implementation of the full recursive algorithm becomes challenging. Such cases demand employment of approximations which helps in reducing the size of the calculations significantly while producing accurate results. We propose and test such approximations. With observation from previous study [34] of disorder enhanced correlations for smaller distances between particles, approximation on the maximum distance between two particles can be applied. Green’s functions with larger distances can be approximated to
Figure 3: Comparison between recursive calculation with that of full diagonalization for two particles in a 2D disordered lattice for $W = 1, V = 1$ (in the unit of hopping) as in Eq. 2 with $\epsilon$ chosen randomly from box distribution $[-W^2, W^2]$. $r = |n - m|$ is the distance between two particles in number of minimum steps in a lattice. Full symbols are for full diagonalization, smaller filled symbols inside are for recursive calculations.

make no contribution to the calculations and hence neglected. This selection of Green’s elements depending on the distance between two particles can also be done dynamically. One can select elements of importance differently at different times of propagation.

$$G(n,m; n', m'; \omega) \simeq 0 \quad \text{for} \quad |n - m| > r$$

(15)

where $r$ is a limiting (Hamming) distance in the number of minimum steps between two particles.
Figure 4: Relative IPR with maximum allowed relative distance $r$ for a small 2D lattice of 12x13 sites. $V = 0$ (left), $V = 4$ (right). IPR calculated in arbitrary scale and averaged over 50 realizations of disorder explain validity of the maximum relative distance approximation.

Figure 4 describes viability of such approximation for calculations of localization parameter IPR of 2D disordered systems. These calculations involved all Green's elements at very large times ($\tau = 1000$) after the approximation applied and computed for a given onsite energy disorder chosen randomly within a uniform distribution of width $W$ ($[-\frac{W}{2}, \frac{W}{2}]$), from particles initially at adjacent sites. The IPR ($\mathcal{I}$) can be calculated from two particle joint densities ($\varrho$), after projecting to single site densities ($\rho$) at time $\tau$.

$$\varrho(m, n, \tau) = |G(m, n, \tau)|^2,$$

$$\rho(m, \tau) = \frac{1}{2} \sum_{n \neq m} \varrho(m, n, \tau),$$

$$\mathcal{I} = \sum_{m} \rho(m, \tau)^2.$$  

The IPR calculations for disordered 2D systems in Fig. 4 show that the limiting distance can be taken as small as $r = 5$ for results with not so significant errors for a broad range of disorder and interaction strength.

The algorithm, however, is more general and can be applied to systems with a general graph structure shown in Fig. 5 where nodes can be distributed into
Figure 5: A general graph structure permitting the recursive computation of the Green’s functions for interacting particles.

layers with each nodes connected to nodes belonging to nearest neighbor layers and nodes within each layer not connected. Specific examples of such graph structure are binary trees. The structure of the recursive calculations maps directly to binary trees when each level of the branches of the tree is taken as a full vector involved in recursive calculations. These tree structures are also known as the Bethe lattice (with a boundary). The root node ($L = 0$) of the tree splits into two branches of same level ($L = 1$). Each node on these branches splits into two different nodes. Any node within the vectors does not connect to each other by the hamiltonian and each such vectors are connected to nearest neighbor vectors only. The two boundary conditions necessary for the computation of the Green’s functions correspond to the vectors at the highest level on the left and right branches approximated to zero.

The spectral weight of interacting particles on a binary tree can be calculated from Eq. 5. For two particles placed on the same site of $L = 0$ on this graph (with maximum $L = 8$), Fig. 7 describes the spectra. The spectrum shows discontinuous peaks as opposed to continuous spectra in 1D and 2D lattices. With stronger
Figure 6: Binary tree of 4 level. Each level separated between left and right branches. Each level within each branch can be considered as a vector involved in recursive calculation as they are not connected to each other by hamiltonian.

interactions, these peaks tend to merge together and a single continuous spectrum enveloping multiple peaks seems to be emerging. Again, the recursive calculations produce excellent agreement with full diagonalization results.

4. Conclusion

In this article a recursive algorithm has been explained for performing calculations related to two-particle Green’s functions. This algorithm is highly efficient and accurate. The algorithm is particularly useful for calculation of correlation dynamics of interacting particles. Spectral properties can also be calculated for large lattice systems using this algorithm. The generality of the algorithm for application beyond lattice systems to certain graph structures can also be useful. Although, the nearest neighbor lattice models are mainly discussed here, further generalizations of the scheme for long-range lattice models are also available [33, 35].
Figure 7: Spectral weight for two particles located on same site calculated for a binary tree of L=8. For non interacting particles, the spectra has multiple peaks with the highest peak at $E = 0$. For strongly interacting particles, the individual peaks are compacted into one peak.

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