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Efficient computation of lattice Green functions for models with longer range hopping

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Abstract

In two recent papers, we have shown how one-particle and few-particle lattice Green functions can be calculated efficiently for models with only nearest-neighbor hopping, using continued fractions. Here, we show that a similar type of solution is possible for models with longer (but finite) range hopping.

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(Some figures may appear in colour only in the online journal)

1. Introduction

The calculation of lattice Green functions is a task that arises in very many solid-state physics problems. For example, one-particle lattice Green functions are used to study effects of disorder [1, 2] or interfaces [3, 4], or to model mesoscopic devices [5], etc. Few-particle Green functions are needed to understand the stability of bound complexes [6] and to interpret various spectroscopies, such as Auger spectra [7].

At the simplest level, assuming a lattice with one state per lattice site and dynamics governed by some model Hamiltonian \mathcal{H} , the one-particle Green functions

$$G(\mathbf{n}, \mathbf{m}, z) = \langle \mathbf{n} | \hat{G}(z) | \mathbf{m} \rangle \quad (1)$$

are matrix elements of the resolvent $\hat{G}(z) = 1/(z - \mathcal{H})$ between states with the particle at sites \mathbf{n} and \mathbf{m} . Usually, $z = E + i\eta$ is a complex number with an infinitesimally small and positive imaginary part, although in certain cases, the presence of non-trivial self-energies may require the Green functions to be calculated away from the real axis.

In a clean system, where invariance to translations holds, the one-particle eigenstates have well-defined momentum $\mathcal{H}|\mathbf{k}\rangle = \epsilon(\mathbf{k})|\mathbf{k}\rangle$ and the lattice Green functions can be expressed as

$$G(\mathbf{n}, \mathbf{m}, z) = \frac{1}{N} \sum_{\mathbf{k}} \frac{\langle \mathbf{n} | \mathbf{k} \rangle \langle \mathbf{k} | \mathbf{m} \rangle}{z - \epsilon(\mathbf{k})}, \quad (2)$$

where N is the number of sites in the lattice, and the sum is over the quasi-momenta in the Brillouin zone consistent with the boundary conditions. For an infinite lattice, $N \rightarrow \infty$ and the sum turns into Fourier transforms. Their direct numerical evaluation is quite cumbersome, especially in higher dimensions, so even in this simplest possible case the calculation is rather hard. If disorder or other complications are present, this approach based on a Lehmann decomposition over the eigenstates becomes that much harder to implement numerically in an efficient way.

The preferred alternative, currently, is the use of the recursion method reviewed in [8], which is linked to the Lanczos method [9]. Briefly, to find $\langle u_0 | \hat{G}(z) | u_0 \rangle$ one uses iterations $\mathcal{H}|u_n\rangle = b_n^*|u_{n-1}\rangle + a_n|u_n\rangle + b_{n+1}|u_{n+1}\rangle$ to generate the orthonormal vectors $\{|u_n\rangle\}$ starting from $|u_0\rangle$ and to calculate the constants $\{a_n\}$, $\{b_n\}$. Because in this basis, \mathcal{H} is a tridiagonal matrix, the matrix element of its resolvent is found to be

$$\langle u_0 | \hat{G}(z) | u_0 \rangle = \frac{1}{z - a_0 - \frac{|b_1|^2}{z - a_1 - \dots}}. \quad (3)$$

To find $G(\mathbf{n}, \mathbf{n}, z)$ one chooses $|u_0\rangle = |\mathbf{n}\rangle$. To find off-diagonal $G(\mathbf{n}, \mathbf{m}, z)$ values, one performs two calculations for $|u_0^{(\pm)}\rangle = |\mathbf{n}\rangle \pm |\mathbf{m}\rangle$. The disadvantage, in this case, is that one may need to work with quite large matrices. As a simple illustration, suppose that we need to calculate the Green function $\langle 0 | \hat{G}(z) | 100 \rangle$ between states at sites 0 and 100, in a one-dimensional (1D) system. Suppose, also, that there is only nearest-neighbor hopping. If $|u_0\rangle \sim |0\rangle + |100\rangle$, then $|u_1\rangle \sim |-1\rangle + |1\rangle + |99\rangle + |101\rangle$, $|u_2\rangle \sim |-2\rangle + |2\rangle + |98\rangle + |102\rangle$, and so on and so forth. One needs to apply the recurrence at least 50 times so that the ‘wave’ started at the origin overlaps at least once with the ‘wave’ originated at site 100. This implies that vectors of at least dimension 200 must be considered, although for accurate values one may well need to go higher. For a different pair of sites, the calculation must be restarted from scratch. Moreover, the problem is obviously compounded in higher dimensions and/or for longer range hopping.

Recently, we introduced a more efficient alternative for calculating lattice Green functions using continued fractions of matrices. It applies to both one-particle [10] and few-particle [6] Green functions for lattices in any dimension, but so far it has been restricted to Hamiltonians with only nearest-neighbor hopping. Here we show that it can be straightforwardly generalized to models with longer (but finite) range hopping. The main result is that we can reduce recurrence relations linking many consecutive terms, to recurrence relations linking only three consecutive quantities. The latter can be solved straightforwardly with continued fractions. The method is useful not only to calculate lattice Green functions, but also for a variety of other problems that can be cast in terms of recurrence relations, such as those reviewed in [11].

2. The method

For simplicity, we first discuss the method in detail for a 1D chain with a single particle. Generalizations to higher dimensions and/or more particles are briefly reviewed next. Continuing to assume a single state per lattice site (multiple states, including spin, are straightforward generalizations), the most general such model Hamiltonian is

$$\mathcal{H} = \sum_n \epsilon_n c_n^\dagger c_n - \sum_{n,m} [t_{n,m} c_n^\dagger c_m + \text{h.c.}],$$

where the first term describes the on-site energies of these states, and the latter the hopping between states located at any sites n and m .

We generate the equations of motion for Green functions by taking the matrix elements of the identity $\hat{G}(z)(z - \mathcal{H}) = 1$, to find $(z - \epsilon_m)G(n, m, z) = \delta_{n,m} - \sum_{m'} t_{m',m} G(n, m', z)$. For any

specified value of n , this can be viewed as a linear system in the unknowns $u_m \equiv G(n, m, z)$. For a small chain, this system can be solved by brute force; however, for an infinite system other approaches are needed.

For nearest-neighbor hopping, an alternative solution is easy since the equations of motion are recurrence relations linking three consecutive terms: $(z - \epsilon_m)G(n, m, z) = \delta_{n,m} - t_{m+1,m}G(n, m + 1, z) - t_{m-1,m}G(n, m - 1, z)$. Just like for the tridiagonal matrices of Haydock's method [8], one can here show that for $m > n$, $G(n, m, z) = A_m(z)G(n, m - 1, z)$, where $A_m(z) = -t_{m-1,m}/[z - \epsilon_m + t_{m+1,m}A_{m+1}(z)]$ is a continued fraction that starts with $\lim_{m \rightarrow \infty} A_m(z) = 0$ (of course, in practice one chooses a sufficiently large cutoff to truncate). Similarly, for any $m < n$, $G(n, m, z) = B_m(z)G(n, m + 1, z)$, where now $B_m(z) = -t_{m+1,m}/[z - \epsilon_m + t_{m-1,m}B_{m-1}(z)]$ and $\lim_{m \rightarrow -\infty} B_m(z) = 0$. As a result, the equation for $n = m$ allows us to find $G(n, n, z) = [z - \epsilon_n + t_{n+1,n}A_{n+1}(z) + t_{n-1,n}B_{n-1}(z)]^{-1}$. From this, all other matrix elements $G(n, m, z)$, $m \neq n$, can then be generated. For a clean system, an analytical solution is possible since the continued fraction can be solved explicitly (for details, see for example [6]).

Previously, we have shown that this solution generalizes to one-particle Green functions in higher dimensions [10] using the idea of a 'Manhattan distance' that is changed by at most 1 through nearest-neighbor hopping. This allows the equations of motion to be grouped as matrix recurrence relations involving only three consecutive terms, and therefore can be solved by a direct generalization in terms of continued fractions of matrices. The same underlying idea also works for few-particle Green functions—in this case, the grouping is done based on a 'relative distance' between the particles, defined such that nearest-neighbor hopping only changes it by ± 1 or 0—preserving the simple recurrence relations structure.

It turns out that a similar philosophy can be used to solve models with longer (but finite) range hopping. To illustrate the idea most simply, consider a 1D Hamiltonian that also has second nearest-neighbor hopping. In this case, the recurrence relations read $(z - \epsilon_m)G(n, m, z) = \delta_{n,m} - t_{m+2,m}G(n, m + 2, z) - t_{m+1,m}G(n, m + 1, z) - t_{m-1,m}G(n, m - 1, z) - t_{m-2,m}G(n, m - 2, z)$. Consider first the $m > n$ equations. We can couple together the equations corresponding to $m = n + 2p$ and $m + 1 = n + 2p + 1$, where $p \geq 1$, in the matrix form:

$$\gamma_p \cdot W_p = \alpha_p \cdot W_{p-1} + \beta_p \cdot W_{p+1}, \tag{4}$$

where

$$W_p \equiv \begin{pmatrix} G(n, m + 2p, z) \\ G(n, m + 2p + 1, z) \end{pmatrix},$$

while

$$\gamma_p \equiv \begin{pmatrix} z - \epsilon_{n+2p} & t_{n+2p+1, n+2p} \\ t_{n+2p, n+2p+1} & z - \epsilon_{n+2p+1} \end{pmatrix},$$

$$\alpha_p \equiv \begin{pmatrix} -t_{n+2p-2, n+2p} & -t_{n+2p-1, n+2p} \\ 0 & -t_{n+2p-1, n+2p+1} \end{pmatrix}$$

and

$$\beta_p \equiv \begin{pmatrix} -t_{n+2p+2, n+2p} & 0 \\ -t_{n+2p+2, n+2p+1} & -t_{n+2p+3, n+2p+1} \end{pmatrix}.$$

Since equation (4) links three consecutive quantities, it can be solved in terms of continued fractions of 2×2 matrices, i.e. for any $p \geq 1$, $W_p = A_p(z) \cdot W_{p-1}$, where $A_p(z) = [\gamma_p - \beta_p \cdot A_{p+1}(z)]^{-1} \alpha_p$, with a cutoff $\lim_{p \rightarrow \infty} A_p(z) = 0$. As a result, using $p = 1$ one can express

$$\begin{pmatrix} G(n, n + 2, z) \\ G(n, n + 3, z) \end{pmatrix} = A_1(z) \cdot \begin{pmatrix} G(n, n, z) \\ G(n, n + 1, z) \end{pmatrix}.$$

A similar regrouping into simple recurrence relations allows one to find

$$\begin{pmatrix} G(n, n-2, z) \\ G(n, n-3, z) \end{pmatrix} = B_1(z) \cdot \begin{pmatrix} G(n, n, z) \\ G(n, n-1, z) \end{pmatrix},$$

where the 2×2 continued fractions $B_p(z)$ are defined quite similarly to the $A_p(z)$. These last relations are then used to turn the equations of motion for $m = n, n \pm 1$ into a system of three linear equations with three unknowns, namely $G(n, n, z)$ and $G(n, n \pm 1, z)$, which can be solved trivially. Once these three Green functions are known, one can generate any desired $G(n, m, z)$ with $m \neq n$ from them using the matrices $A_p(z), B_p(z)$.

3. Results

We demonstrate this method for several simple cases, with no disorder, where the results can be easily checked against results obtained by brute-force integration.

3.1. One particle on a 1D clean chain

For a clean chain, we can set $\epsilon_n \equiv 0, t_{n,n+1} = t$ and $t_{n,n+2} = t'$. The invariance to translations implies that $G(n, m, z) = G(m-n, z) = G(n-m, z) \rightarrow u_{|m-n|}$, so we can choose $n = 0$ and only consider positive m (or p) values. Moreover, in the absence of disorder all the matrices become independent of p and therefore $A_p(z) \rightarrow A(z)$ which satisfies

$$[\gamma - \beta A(z)]A(z) = \alpha, \tag{5}$$

where, in terms of Pauli and the identity matrices, $\alpha = -t' - t\sigma_+/2, \beta = -t' - t\sigma_-/2$ and $\gamma = z + t\sigma_x$.

Not surprisingly, equation (5) has multiple solutions. The reason for this is easy to understand. This equation only encodes the recurrence relation $zu_n = -t(u_{n+1} + u_{n-1}) - t'(u_{n+2} + u_{n-2})$. Its general solution is of the form $u_n = \sum_{\alpha=1}^4 c_\alpha \zeta_\alpha^n$, where ζ_α are the four roots of the characteristic equation $t'(\zeta^4 + 1) + t(\zeta^3 + \zeta) + z\zeta^2 = 0$. For any finite value of η , two of these roots have absolute values below unity, and two of them are larger than 1. The eigenvalues of the matrices $A(z)$ which satisfy equation (5) can correspond to any two of these four possible roots; hence, the many possible solutions. (To be more precise, if λ_1 and λ_2 are the eigenvalues of $A(z)$, then its general solution for the recurrence equation is of the form $u_{2n} = a_1\lambda_1^n + b_1\lambda_2^n, u_{2n+1} = a_2\lambda_1^n + b_2\lambda_2^n$, where $(a_1 a_2)^T$ and $(b_1 b_2)^T$ are the right eigenvectors of $A(z)$, up to some overall constants. Comparing this with the general solution given above, it follows that $\lambda_1 = \zeta_i^2$ for some value of $i = 1, 4$, and similarly $\lambda_2 = \zeta_j^2$, for some other $j \neq i$.)

The actual physical solution, i.e. the values of the coefficients $c_\alpha, \alpha = 1, 4$, is fixed by how the set of recurrence relations is started near the origin: $zu_0 = 1 - 2tu_1 - 2t'u_2$ and $zu_1 = -t(u_0 + u_2) - t'(u_1 + u_3)$. (We used explicitly the symmetries $G(0, 1, z) = G(0, -1, z) \rightarrow u_1$ etc.) What we know for certain is that the physical solution must vanish as $n \rightarrow \infty$. This is because its Fourier transform is proportional to the amplitude of probability for the particle to travel a distance n within a time τ . This must always vanish for a sufficiently large n , because the small η is equivalent to a finite lifetime for the particle, and this prevents it from traveling arbitrarily far in a finite amount of time. As a result, the physical solution will only contain the two roots whose modulus is less than unity. Computationally, it can be found by iterations starting with $A = 0$, which are equivalent to propagating a solution from large n toward the origin. This naturally selects the physical roots (the unphysical roots are exponentially suppressed) and thus the correct form for $A(z)$ (for more discussion, see [6] or [12]).

To find the solutions once $A(z)$ is known, we use the two equations near the origin. The end result is

$$\begin{pmatrix} G(0, 0, z) \\ G(0, 1, z) \end{pmatrix} = M(z) \cdot \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad (6)$$

where

$$M(z) = \left[\begin{pmatrix} z & 2t \\ t & z+t' \end{pmatrix} + \begin{pmatrix} 2t' & 0 \\ t & t' \end{pmatrix} \cdot A(z) \right]^{-1}.$$

All other Green functions can then be obtained by multiplying with $A(z)$ repeatedly.

Since we know how to generate the physical solution $A(z)$ using iterations, we can compare it to the various possible analytical solutions and select the correct one, namely

$$A(z)|_{11} = 1 - \frac{s(z)(\sqrt{s(z)+4t'} - \sqrt{s(z)-4t'})^2}{16t'^2}, \quad (7)$$

$$A(z)|_{12} = -\frac{(\sqrt{t+a(z)} - \sqrt{t-a(z)})^2}{4t'}, \quad (8)$$

$$A(z)|_{21} = \frac{1}{4t'^2} \left(\frac{[\sqrt{t+a(z)} - \sqrt{t-a(z)}]^2 ([s(z)]^2 - 4t'^2)}{4t'} - 4tt' \right), \quad (9)$$

$$A(z)|_{22} = 1 - \frac{1}{4tt'^2} \left[t[a(z)]^2 - [\sqrt{t+a(z)} - \sqrt{t-a(z)}]^2 \left(t^2 - \frac{[s(z)]^2}{4} \right) \right], \quad (10)$$

where

$$a(z) = [\sqrt{t'(z+2t+2t')} - \sqrt{t'(z-2t+2t')}]$$

and

$$s(z) = [\sqrt{t'(z+2t+2t')} + \sqrt{t'(z-2t+2t')}]^2.$$

Together with equation (6), this gives the analytical solution for Green functions of this problem for the first time to the best of our knowledge. As a validation of these results, figure 1 shows the total density of states $\rho(E) = -\frac{1}{\pi} \text{Im} G(0, 0, z)$ obtained from this analytical solution (lines) versus results obtained by the direct numerical integration of equation (2) (symbols). The agreement is excellent, as expected.

As discussed above, the method can be used for disordered systems, using continued fractions to evaluate the various $A_p(z), B_p(z)$, starting from sufficiently large cutoffs. The generalization to longer (but finite) range hopping is straightforward as well, and simply requires grouping together more Green functions within each W_p . With the proper grouping, the equations of motion can always be recast as recurrence relations between three consecutive vectors W_{p-1}, W_p and W_{p+1} , and solved with continued fractions.

3.2. One particle on a two-dimensional square lattice

For simplicity, we illustrate this example for a clean square lattice and assume that only nearest-neighbor and second nearest-neighbor hoppings are allowed. Again, only the relative distance is relevant, since $G(\mathbf{n}, \mathbf{m}; z) = G(\mathbf{n} - \mathbf{m}; z) = G(\mathbf{m} - \mathbf{n}; z) \rightarrow u_{\mathbf{m}-\mathbf{n}}$ etc. The resulting equations of motion read $zu_{n_x, n_y} = \delta_{n_x, 0} \delta_{n_y, 0} - t(u_{n_x+1, n_y} + u_{n_x-1, n_y} + u_{n_x, n_y+1} + u_{n_x, n_y-1}) - t'(u_{n_x+1, n_y+1} + u_{n_x+1, n_y-1} + u_{n_x-1, n_y+1} + u_{n_x-1, n_y-1})$. At first sight, this is not a simple recurrence relation even for $t' = 0$. However, it can be recast as one in terms of the vectors V_N which include all distinct Green functions for which the ‘Manhattan distance’ is $|n_x| + |n_y| = N$. It

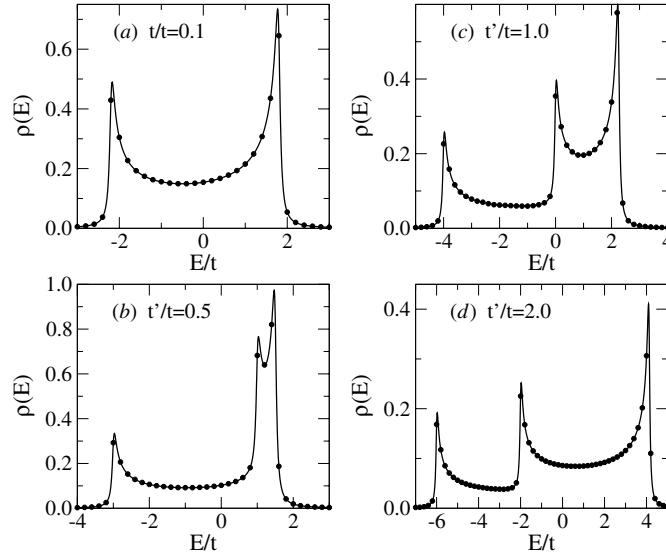


Figure 1. Density of states $\rho(E) = -\frac{1}{\pi} \text{Im} G(0, 0, E + i\eta)$ versus E , for a particle on a clean 1D chain with the nearest-neighbor t and second nearest-neighbor hopping t' . The parameters are $t'/t = 0.1, 0.5, 1.0$ and 2.0 , respectively, and $\eta = 0.05$. The lines show the analytical results of equations (6)–(10), while the circles are obtained by the numerical integration of equation (2).

is then straightforward to check that the nearest-neighbor hopping only links the elements of V_N to the elements of $V_{N\pm 1}$, and the continued-fraction method can be used [10]. Clearly, if the second nearest-neighbor hopping is turned on as well, then the elements of V_N will also be linked to the elements of $V_{N\pm 2}$. Using the same approach as before, i.e. grouping together all the elements of V_{2N} and V_{2N+1} within a bigger vector W_N , ensures that W_{N-1}, W_N, W_{N+1} are linked through matrix recurrence relations that can be solved in terms of continued fractions of matrices.

Results for several values of t'/t are shown in figure 2. The lines are the results obtained by our continued-fraction method, while the symbols are obtained from equation (2). The agreement is excellent, even for a rather small cutoff in the Manhattan distance of $N_{\text{max}} = 100$. What value needs to be used for this cutoff depends on various parameters. Inside the band, the value increases with decreasing η , while outside the spectrum convergence is always very fast. As an example, in figure 3 we show data for the same η , but a smaller cutoff $N_{\text{max}} = 40$. Clearly, here the results are not yet fully converged. Additional discussion on the interplay between N_{max} and η is available in [6]. While we find that for any value of η , the results eventually converge if N_{max} is sufficiently large, it would be useful to know if more efficient ways of truncating the continued fraction (than setting it to zero) exist. We are not aware of a general method for identifying these, although one can find such schemes in particular cases, as exemplified in [10].

While we used the square lattice here for simplicity, the generalization to higher dimensions and/or other types of lattices is possible, following the lines discussed in [10] for nearest-neighbor only hopping.

3.3. Three spinless fermions on a one-dimensional clean chain

Finally, we illustrate the implementation of the method for the simplest non-trivial few-particle Green functions model, namely for three spinless fermions on a 1D chain, with

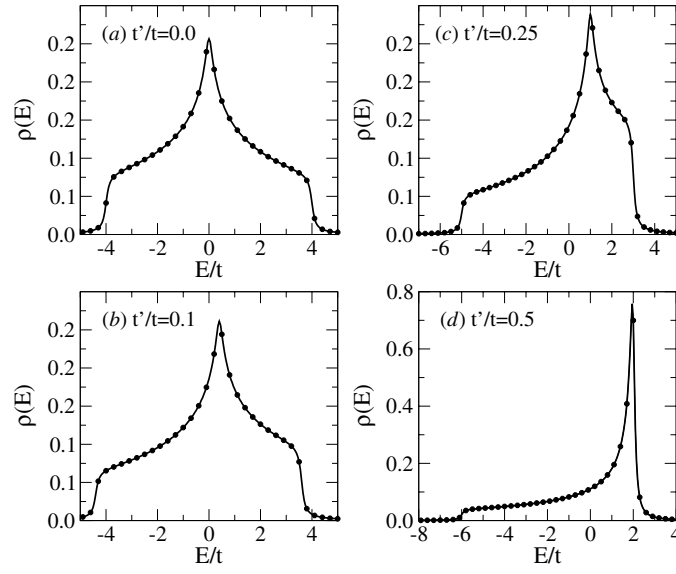


Figure 2. Local density of states $\rho(E) = -\frac{1}{\pi} \text{Im} G(0, 0, E + i\eta)$ versus E , for a particle on a clean square lattice with the nearest-neighbor hopping t and second nearest-neighbor hopping t' . The parameters are $t'/t = 0.0, 0.1, 0.25$ and 0.5 , respectively, $\eta = 0.1$ and the cutoff is $N_{\text{max}} = 100$. The lines show the results of our method, while the circles are obtained using equation (2).

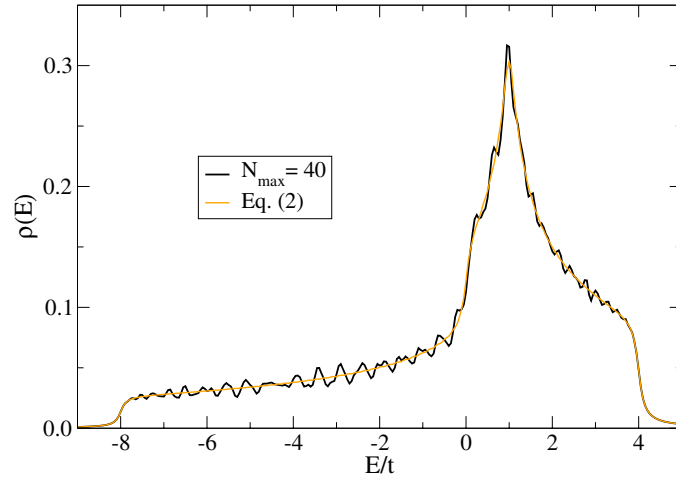


Figure 3. Same density of states $\rho(E)$ as in figure 2 for $t' = t$ and a cutoff $N_{\text{max}} = 40$. Clearly, convergence has not yet been reached for our continued-fraction method.

nearest-neighbor and second nearest-neighbor hoppings t and t' , and nearest-neighbor and second nearest-neighbor interactions U_1 and U_2 , respectively:

$$\mathcal{H} = \sum_i [-t c_i^\dagger c_{i+1} - t' c_i^\dagger c_{i+2} + \text{h.c.}] + \sum_i [U_1 n_i n_{i+1} + U_2 n_i n_{i+2}], \quad (11)$$

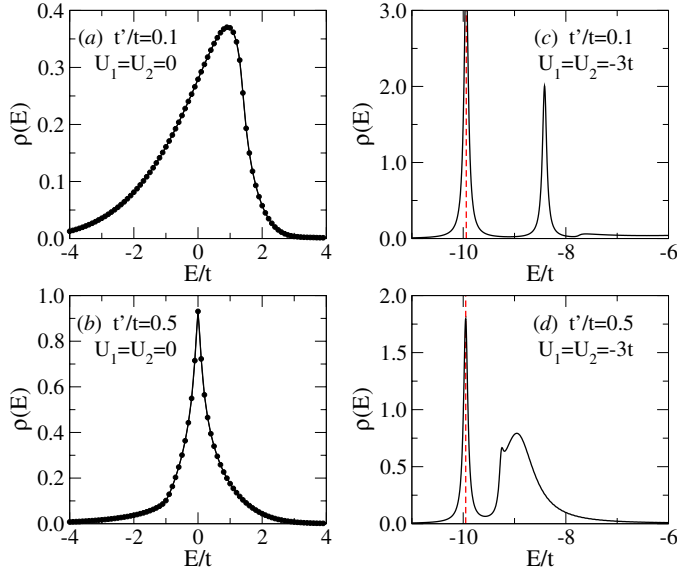


Figure 4. Density of states $\rho(\omega) = -\frac{1}{\pi} \text{Im} G(k = 0; 1, 1; 1, 1; E + i\eta)$ versus E for (a) $U_1 = U_2 = 0, t'/t = 0.1$; (b) $U_1 = U_2 = 0, t'/t = 0.5$; (c) $U_1 = U_2 = -3t, t'/t = 0.1$; (d) $U_1 = U_2 = -3t, t'/t = 0.5$. Full lines show our results, for a cutoff $N_{\text{max}} = 100$ and $\eta = 0.05$. Circles in (a) and (b) are results of direct integration, while the dashed lines in (c) and (d) mark the expected location of the trion bound state for $k = 0$, as obtained from exact diagonalization for a chain with 30 sites.

where $n_i = c_i^\dagger c_i$. Because the model is invariant to translations, the total momentum is a good quantum number and therefore it is convenient to work with states of the form

$$|k, n_1, n_2\rangle = \frac{1}{\sqrt{N}} \sum_i e^{ikR_i} c_{i-n_1}^\dagger c_i^\dagger c_{i+n_2}^\dagger |0\rangle,$$

with $n_1 \geq 1, n_2 \geq 1$ to avoid double counting. The corresponding three-particle Green functions are $G(k; n_1, n_2; m_1, m_2; z) = \langle k, n_1, n_2 | \hat{G}(z) | k, m_1, m_2 \rangle$. Suppose we are interested in the case $n_1 = n_2 = 1$. Their equations of motion are straightforward but too long and cumbersome to write down. In any event, if $t' = 0$, they can be recast as simple recurrence relations between the vectors V_{N-1}, V_N and V_{N+1} , where V_N contains all Green functions for which $m_1 + m_2 = N$, see [6]. Turning on t' will mix $V_{N\pm 2}$ in these recurrence relations, but they can be turned into simple recurrence relations for vectors W_N which include all V_{2N}, V_{2N+1} entries, like in the other cases discussed.

We have checked this solution in several ways. First, if $U_1 = U_2 = 0$, then the fermions are non-interacting. Eigenstates with the total momentum k are of the general form $c_{k-k_1-k_2}^\dagger c_{k_1}^\dagger c_{k_2}^\dagger |0\rangle$ and have eigenenergy $\epsilon(k - k_1 - k_2) + \epsilon(k_1) + \epsilon(k_2)$, where $\epsilon(k) = -2t \cos(k) - 2t' \cos(2k)$. The Lehmann representations for the lattice Green functions then involve two integrals over the Brillouin zone, over k_1 and k_2 , and can be evaluated numerically. As an example, in figures 4(a) and (b) we compare our result (line) against the one computed from the Lehmann representation (symbols) for $k = 0$ and $t'/t = 0.1, 0.5$. The agreement is excellent. Another check is for finite U_1 and U_2 but $t' = 0$ —in this case, the results agree with those of [6] (not shown).

Finally, for finite t'/t and non-vanishing interactions, we look at cases where U_1 and U_2 are sufficiently attractive so that a trion (a bound three-particle complex) is formed, and compare its energy against that obtained for $k = 0$ using a full diagonalization for a 30-site chain using LAPACK. Typical results are shown in figures 4(c) and (d). The trion energy obtained from LAPACK is marked by the dashed line, and is in good agreement with the location of the lowest peak in our density of states (full line).

The few examples and results given here should suffice to validate our method. Generalizations to more complicated cases are straightforward.

4. Conclusions

In conclusion, we have shown that the continued-fraction method can be used to calculate both one-particle and few-particle lattice Green functions in any dimension and essentially for any type of hopping, as long as it is finite-ranged. Our results should be useful for a multitude of problems which require such lattice Green functions as an input to obtaining other quantities.

More generally, our method illustrates how recurrence relations linking more than three consecutive terms can be reduced to simple recurrence relations linking only three consecutive quantities. Since a much wider class of physics problems can be cast in such terms, we believe that this idea will have widespread applications.

Acknowledgments

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References

- [1] Economou E N 1983 *Green's Functions in Quantum Physics* (Berlin: Springer)
- [2] Gonis A 1992 *Green Functions for Ordered and Disordered Systems* (New York: Elsevier)
- [3] Einstein T L and Schrieffer J R 1973 Indirect interaction between adatoms on a tight-binding solid *Phys. Rev. B* **7** 3629
- [4] Molina M I 2005 Nonlinear surface impurity in a semi-infinite lattice *Phys. Rev. B* **71** 035404
- [5] Datta S 1977 *Electronic Transport in Mesoscopic Systems* (Cambridge: Cambridge University Press)
- [6] Berciu M 2011 Few-particle Green's functions for strongly correlated systems on infinite lattices *Phys. Rev. Lett.* **107** 246403
- [7] Sawatzky G A 1977 Quasiatomic Auger spectra in narrow-band metals *Phys. Rev. Lett.* **39** 504
- [8] Haydock R, Heine V and Kelly M J 1975 Electronic structure based on the local atomic environment for tight-binding bands: II *J. Phys. C: Solid State Phys.* **8** 2591
- [9] Lanczos C 1950 An iteration method for the solution of the eigenvalue problem of linear differential and integral operators *J. Res. Natl Bur. Stand.* **45** 255
- [10] Berciu M and Cook A M 2010 Efficient computation of lattice Green's functions for models with nearest-neighbour hopping *Europhys. Lett.* **92** 40003
- [11] Cini M and D'Andrea A 1988 Exactly solved electron-boson models in condensed matter and molecular physics by a generalized recursion method *J. Phys. C: Solid State Phys.* **21** 193
- [12] Berciu M 2009 On computing the square lattice Green's function without any integrations *J. Phys. A: Math. Theor.* **42** 395207