

# On computing the square lattice Green's function without any integrations

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## Abstract

We extend Morita's work on lattice Green's functions (1971 *J. Math. Phys.* **12** 1744) and show that in principle, all Green's functions  $G(n, m, \omega)$  for a square lattice can be calculated using continued fractions, with no need for any integrations. In reality, this method gives highly accurate values if  $|n| - |m|$  is a small integer, however for larger differences numerical computational errors render the results untrustworthy, like for the original Morita scheme. The method proposed here can be generalized to a much wider class of special functions related by recurrence relations.

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(Some figures in this article are in colour only in the electronic version)

## 1. Introduction

Consider the nearest-neighbor hopping Hamiltonian on a square lattice,

$$\mathcal{H} = -t \sum_{i,j} \left[ c_{i,j}^\dagger (c_{i,j+1} + c_{i+1,j}) + \text{h.c.} \right], \quad (1)$$

and Green's function associated with it,

$$G(n, m, \omega) = \langle 0 | c_{i+n, j+m} \frac{1}{\omega - \mathcal{H} + i\eta} c_{i,j}^\dagger | 0 \rangle, \quad (2)$$

where  $c_{i,j}$  is the annihilation operator for a particle at site  $(i, j)$  (we used the invariance to translations of the Hamiltonian to remove dependence of  $i, j$  in equation (2), and we take  $\hbar = 1$ ). The need to evaluate  $G(n, m, \omega)$  arises in a multitude of contexts in condensed matter problems. The solution in terms of a double integral is trivial to write

$$G(n, m, z) = \frac{1}{t(2\pi)^2} \int_{-\pi}^{\pi} dx \int_{-\pi}^{\pi} dy \frac{e^{inx+imy}}{z + 2 \cos x + 2 \cos y}, \quad (3)$$

where we define  $z = (\omega + i\eta)/t$  and from now on we take  $t = 1$  as the unit of energy. Also, we only consider the case  $0 \leq m \leq n$ , since all other values are obtained from symmetries given that  $G(\pm m, \pm n, z) = G(\pm n, \pm m, z)$ , etc. One of the two integrals in equation (3) can be evaluated analytically but the second must be computed numerically. This can be time consuming, especially if one needs many results corresponding to large values of  $n$  and  $m$ , where the integrand is a strongly oscillating function.

In [1], Morita derived recurrence relations for the diagonal Green's functions with  $n = m \geq 1$ , namely

$$G(n + 1, n + 1, z) = \frac{4n}{2n + 1} \left( \frac{z^2}{8} - 1 \right) G(n, n, z) - \frac{2n - 1}{2n + 1} G(n - 1, n - 1, z). \quad (4)$$

While in [1] this relation was derived using elementary integrations by parts, more recently it was revealed that Green's functions with  $n = m$  are linked to certain hypergeometric functions [2] and even to wavelets [3]. These connections would enable us to generalize the discussion that follows; however, for clarity, we will focus on the square lattice Green's functions in this work.

Morita argued that using equation (4) together with the equation of motion

$$zG(n, m, z) + G(n + 1, m, z) + G(n - 1, m, z) + G(n, m + 1, z) + G(n, m - 1, z) = \delta_{n,0}\delta_{m,0} \quad (5)$$

allows one to compute all  $G(n, m, z)$  based on knowing just

$$A(z) = G(0, 0, z) = \frac{2}{\pi z} K\left(\frac{4}{z}\right),$$

$$B(z) = G(1, 1, z) = \frac{2}{\pi z} \left( \frac{z^2}{8} - 1 \right) K\left(\frac{4}{z}\right) - \frac{z}{4\pi} E\left(\frac{4}{z}\right). \quad (6)$$

In other words, only two elliptical integrals need to be evaluated explicitly to find  $A(z)$  and  $B(z)$ ; then equation (4) allows one to calculate all  $G(n, n, z)$  with  $n \geq 2$ , from which using equation (5) and symmetries one can derive all other  $G(n, m, z)$ ,  $0 \leq m < n$ . Furthermore, these values can then be used for the efficient calculation of various three-dimensional lattice Green's functions.

While in principle correct, in practice Morita's method has to be used with caution, because it can easily give wrong answers due to unavoidable computational errors. This is especially so if one is interested in fairly large values of  $n$ , and/or in frequencies outside the free-particle continuum  $|\omega| = |\text{Re}z| > 4$ , and/or a large value of the broadening  $\eta = \text{Im}z$  (the latter may be the case if the energy is renormalized by a self-energy that has a finite imaginary part). The reason is easy to understand: like many recurrence relations, that of equation (4) has a solution that increases exponentially and one that decreases exponentially as  $n \rightarrow \infty$  (more details and specific examples are provided below). The physical solution is the one that decreases exponentially. This is obvious outside the free-particle band  $|\omega| = |\text{Re}z| \geq 4$ , but is true inside the continuum also as long as  $\eta = \text{Im}z$  remains finite (which is always the case in numerical calculations). Unless  $A(z)$  and  $B(z)$  are evaluated with infinite accuracy—which is impossible due to truncation errors, at the very least—the unphysical solution is not eliminated by the initial conditions and it starts to grow very fast and dominate the answer as  $n$  increases and the correct physical solution becomes exponentially small.

In this paper, we show that one can evaluate  $G(n, n, z)$  for arbitrarily large  $n$  values, with arbitrary accuracy and extremely efficiently, without doing any integrals, in terms of continued fractions. In principle, this approach extends to all other  $G(n, m, z)$  functions, although small computational errors again creep in and ruin the results if  $n - m$  becomes large enough.

The method we propose here allows us not only to evaluate diagonal and near-diagonal lattice Green's functions very easily and accurately, but can be applied to any integrals that are related by recurrence relations similar to equation (4). Since such relations are ubiquitous for many special functions that appear in physics, we believe that this simple method should prove very useful for numerical computations in a much wider context.

## 2. The extreme sensitivity of the Morita solution to errors in $A(z)$ and $B(z)$

One can use Mathematica or similar software to generate the expressions for the various  $G(n, m, z)$  in terms of  $A(z)$  and  $B(z)$ , according to the Morita scheme described above. A few of these expressions are listed, for instance, in [4], and they look like very simple and well-behaved polynomials in  $z$ ,  $A(z)$  and  $B(z)$ . For instance,

$$G(3, 0, z) = \frac{1}{4} + z \left( \frac{3A(z)}{4} + 3B(z) + z \left( \frac{1}{4} - \frac{zA(z)}{4} \right) \right), \quad (7)$$

while

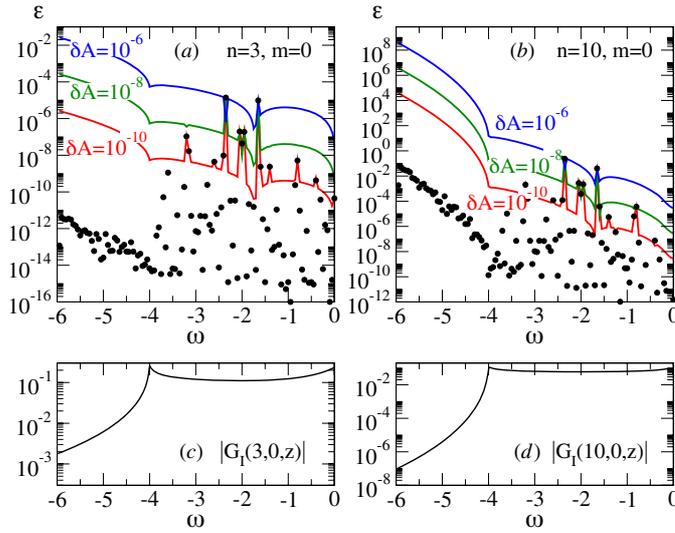
$$\begin{aligned} G(10, 0, z) = & -\frac{811A(z)}{315} - \frac{1126B(z)}{315} + z \left( -\frac{25}{4} + z \left( -\frac{67751A(z)}{420} - \frac{99118B(z)}{315} \right. \right. \\ & + z \left( -100 + z \left( -\frac{21991A(z)}{105} - \frac{54399B(z)}{70} + z \left( -\frac{441}{4} + z \left( \frac{66233A(z)}{1260} - \frac{63793B(z)}{315} \right. \right. \right. \\ & \left. \left. \left. + z \left( -16 + z \left( 15A(z) - \frac{7129B(z)}{1260} + z \left( -\frac{1}{4} + \frac{zA(z)}{4} \right) \right) \right) \right) \right) \right) \right). \quad (8) \end{aligned}$$

Note that in [4] the unit of energy is chosen to be  $t = 1/4$  and that changes the expressions for  $G(n, m, z)$  accordingly. Once the desired value of  $z$  is chosen, there are two main sources of errors in expressions like equations (7) and (8). The first is due to errors in the values of  $A(z)$  and  $B(z)$ , coming from the numerical evaluation of the integrals appearing in equation (6). The second is due to numerical errors when evaluating the polynomials that multiply  $A(z)$  and  $B(z)$  in these expressions, and can be especially severe when large terms with opposite signs are added together, as is often the case. We now estimate the sensitivity to the first type of error.

The dots in figure 1 show the relative error  $\epsilon = |1 - G_M(n, m, z)/G_I(n, m, z)|$  in the value of Green's function as estimated by the Morita scheme,  $G_M(n, m, z)$ , versus direct numerical integration,  $G_I(n, m, z)$ <sup>1</sup>, as a function of  $\omega = \text{Re}z$ . Panel (a) shows the results for  $n = 3, m = 0$ , while panel (b) corresponds to  $n = 10, m = 0$ . Panels (c) and (d) show  $|G_I(n, m, z)|$  for the two cases, revealing a finite function at all  $z$  values. Given the particle-hole symmetry of the Hamiltonian, it suffices to investigate the  $\omega < 0$  interval. For smaller  $n$  both methods are in very good agreement with relative errors below  $10^{-4}$  everywhere. For  $n = 10$ , though, the agreement is more questionable, with a few discrete points where the relative error is already of order 1. Of course, since neither method is exact, one cannot *a priori* decide which method is at fault, based on these results alone.

To demonstrate the sensitivity of the Morita scheme to small changes in the values of  $A(z)$  and  $B(z)$ , we also show the same quantities when a small change  $\delta A = 10^{-10}, 10^{-8}$  respectively  $10^{-6}$  is added to the computed value of  $A(z)$  (similar results are obtained if the imaginary part of  $A(z)$ , respectively either the real or imaginary parts of  $B(z)$  are thus changed). The relative errors increase, as expected, since the results given by the Morita scheme are now certainly less accurate. For the smaller  $n$  case the increase is minimal,

<sup>1</sup> The numerical integration was carried out using the subroutine dqag from the quadpack library



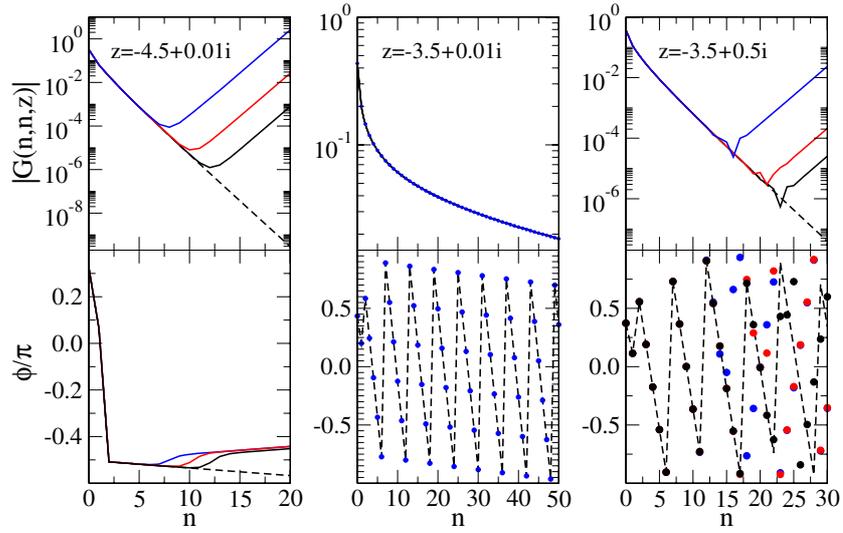
**Figure 1.** Relative error in the value of  $G(n, m, z)$  as estimated by the Morita scheme versus numerical integration (dots). The lines show the same quantity, when an absolute error of  $10^{-10}$ ,  $10^{-8}$  respectively  $10^{-6}$  is added by hand to the value of  $A(z)$  used in the Morita scheme. Here  $z = \omega + i\eta$  and  $\eta = 10^{-2}$ . Panel (a) corresponds to  $n = 3, m = 0$ , while panel (b) to  $n = 10, m = 0$ . Panels (c) and (d) show the value of  $|G(n, m, z)|$  as calculated by numerical integration.

showing limited sensitivity to the values of  $A(z)$  and  $B(z)$  used. For the larger  $n$  value, however, such tiny errors in  $A(z)$  result in tremendous changes in the resulting  $G(n, m, z)$  leading to huge relative errors, or in other words very wrong results.

This extreme sensitivity is most pronounced outside the free particle spectrum  $|\omega| \geq 4$ , and it worsens as  $n$  increases. It is also worsened with increased values of  $\eta$ , even inside the continuum. Energies outside the continuum are of interest for solutions related to all impurity problems [5] as well as momentum average approximations [6], so accurate solutions here are desirable just as much as inside the continuum.

As alluded to in the introduction, the origin of this sensitivity to the values of  $A(z)$  and  $B(z)$  can be traced, at least in part, to the recurrence relation of equation (4). In figure 2 we plot the absolute value (top) and phase (bottom) of  $G(n, n, z)$  calculated with equation (4) (full lines) and by direct numerical integration (dashed lines). The left panels correspond to  $z = -4.5 + 0.01i$ , i.e. an energy outside the continuum. As expected, here Green's function decreases exponentially with distance  $n$ . The Morita solution initially agrees with the numerical integration, however at a larger  $n$  it starts to increase exponentially. The larger the error in either  $A(z)$  or  $B(z)$ , the faster the discrepancy sets in. Such behavior is always seen outside the continuum. Typically, the further away the energy is from the continuum, the smaller the value of  $n$  where the discrepancy sets in and the results obtained from equation (4) are untrustworthy.

The central row of panels corresponds to  $z = -3.5 + 0.01i$ . For this energy inside the continuum, we find excellent agreement between the two solutions, at least up to  $n = 50$ . However, the right set of panels shows that if the imaginary part is not so small, then discrepancies set in again at a fairly small  $n$ . Where precisely this happens depends on the values of  $\omega$ ,  $\eta$  and, of course, the errors in the values of  $A(z)$  and  $B(z)$ . We also note that



**Figure 2.** Top panels: absolute value  $|G(n, n, z)|$  versus  $n$  for three values of  $z$ . Bottom panels: phase of  $G(n, n, z)$  in units of  $\pi$  versus  $n$ , for the same values of  $z$ . The full lines correspond to the Morita solution, while the dashed ones are from direct numerical integration. The red/blue lines are the Morita solution where  $\delta A = 10^{-8}$ , respectively,  $10^{-6}$  was added by hand to  $A(z)$ .

even though the central panels show that the Morita solution is very accurate for  $G(n, n, z)$  if  $z$  corresponds to an energy inside the continuum and a small  $\eta$ , figure 1 shows that even for such cases, significant problems can arise for predicted  $G(n, m, z)$  values as  $n - m$  increases. This suggests that errors accumulate as one increases  $n - m$ , over and above the errors that appear as one increases  $n$ , for  $m = n$ . This is consistent with data that is shown below.

In the limit  $n \rightarrow \infty$ , equation (4) simplifies to

$$G(n + 1, n + 1, z) = 2 \left( \frac{z^2}{8} - 1 \right) G(n, n, z) - G(n - 1, n - 1, z). \quad (9)$$

This recurrence relation has solutions of the general form

$$G(n, n, z) = \alpha(z)[\lambda_+(z)]^n + \beta(z)[\lambda_-(z)]^n, \quad (10)$$

where

$$\lambda_{\pm}(z) = \frac{z^2}{8} - 1 \pm \frac{z}{8} \sqrt{z - 4} \sqrt{z + 4} \quad (11)$$

are the roots of the characteristic polynomial  $\lambda^2 - 2 \left( \frac{z^2}{8} - 1 \right) \lambda + 1 = 0$ . Clearly, these roots are complex conjugate and their product is unity. Moreover, when expressed as in equation (11), they are such that  $|\lambda_-| < 1$ , and therefore  $|\lambda_+| > 1, \forall z$  as long as  $\eta$  is finite.

Thus, in the asymptotic limit  $n \rightarrow \infty$ , we know that the physical solution must be  $G(n, n, z) \sim [\lambda_-(z)]^n$ . This is because Green's function is related to the amplitude of probability for the particle to move a distance of  $(n, n)$  away, and therefore it cannot diverge with  $n$ . This condition implies that we must find  $\alpha(z) = 0$  in equation (10).

The problem with solving equation (4) starting from  $n = 0$ , i.e. from  $A(z) = G(0, 0, z)$  and  $B(z) = G(1, 1, z)$ , is now obvious. If all the values were calculated with infinite precision, equation (4) would ensure that in the asymptotic limit  $\alpha(z) = 0$ , i.e. only the physical solution

is propagated. Any error coming either from the initial values used or incurred as the solution is propagated will result in a  $\alpha(z)$  which is finite. Irrespective of how small it is, as long as it is finite, it will give a solution dominated by the diverging contribution  $\lambda_+^n$  when  $n$  becomes large enough.

### 3. Computational scheme based on continued fraction

The way to fix the problem is clear: the recurrence relation must be used in the other direction, i.e. starting from large  $n$  and moving toward  $n = 0$ . We have just established that as  $n \rightarrow \infty$ , we must have

$$G(n + 1, n + 1, z) = \lambda(z)G(n, n, z), \tag{12}$$

where from now on we use the simplified notation  $\lambda(z) \equiv \lambda_-(z)$ . Inserting this into equation (4) we find that  $G(n, n, z)$  and  $G(n - 1, n - 1, z)$  must also be proportional, and so on all the way to  $n = 0$ . In other words, for any  $n \geq 0$  we must have

$$G(n + 1, n + 1, z) = R_0(n, z)G(n, n, z), \tag{13}$$

where from equation (4) it follows that

$$R_0(n, z) = \frac{\frac{2n+1}{2n+3}}{\frac{4(n+1)}{2n+3} \left( \frac{z^2}{8} - 1 \right) - R_0(n + 1, z)}. \tag{14}$$

All these ratios can be calculated easily starting from  $R_0(n, z) = \lambda(z)$  at a sufficiently large  $n$ . To find the actual values, though, we need to know explicitly one of these Green's functions. To obtain it, we now analyze Green's functions on the next 'diagonal', i.e. the values of  $G(n + 1, n, z)$ .

From the equation of motion (5), we find that for any  $n \geq 1$ ,

$$\frac{z}{2}G(n, n, z) + G(n, n - 1, z) + G(n + 1, n, z) = 0 \tag{15}$$

and therefore

$$\frac{z}{2}G(n + 1, n + 1, z) + G(n + 1, n, z) + G(n + 2, n + 1, z) = 0. \tag{16}$$

Using the proportionality of equation (12) allows us to find a new recurrence relation along this 'diagonal':

$$G(n + 2, n + 1, z) = [R_0(n, z) - 1]G(n + 1, n, z) + R_0(n, z)G(n, n - 1, z). \tag{17}$$

Analyzing the asymptotic limit  $n \rightarrow \infty$  leads again to the conclusion that for any  $n \geq 1$ ,

$$G(n + 1, n, z) = R_1(n, z)G(n, n - 1, z), \tag{18}$$

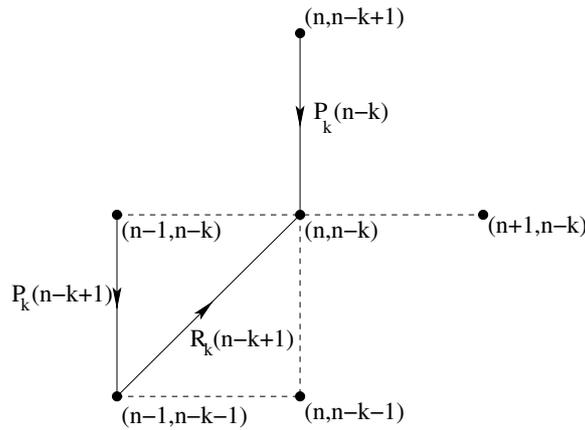
where

$$R_1(n, z) = \frac{R_0(n + 1, z)}{R_1(n + 1, z) - R_0(n + 1, z) + 1} \tag{19}$$

with the asymptotic solution  $R_1(n \rightarrow \infty, z) = \lambda(z)$  (note that the other possible solution,  $R_1(n \rightarrow \infty, z) = 1$ , is not acceptable on physical grounds). Thus, these ratios can be calculated very easily in parallel with calculating the  $R_0(n, z)$  values.

Using equation (18) together with equation (15), we also find that for any  $n \geq 1$ , we must have

$$G_0(n, n - 1, z) = P_1(n - 1, z)G(n, n, z) = -\frac{z}{2[1 + R_1(n - 1, z)]}G(n, n, z); \tag{20}$$



**Figure 3.** Ratios needed to express  $G(n, n-k+1, z)$  and  $G(n-1, n-k, z)$  in terms of  $G(n, n-k, z)$  (see the text for details).

in other words, these ratios are also known. We are now ready to find the reference values, by using the equation of motion for  $n = m = 0$ :

$$zG(0, 0, z) + 4G(1, 0, z) = 1. \tag{21}$$

Together with  $G(1, 0, z) = P_1(0, z)G(1, 1, z) = P_1(0, z)R_0(0, z)G(0, 0, z)$  which follows from combining equations (20) and (13), we find

$$G(0, 0, z) = \frac{1}{z + 4P_1(0, z)R_0(0, z)}; \quad G(1, 0, z) = \frac{4P_1(0, z)R_0(0, z)}{z + 4P_1(0, z)R_0(0, z)}. \tag{22}$$

With these two reference values and all the consecutive ratios in hand, we can now generate all values along the two diagonals, i.e all  $G(n, n, z)$  and  $G(n + 1, n, z)$  of interest, without having done any integrals.

This approach can be generalized to all other ‘diagonals’. Indeed, we assume that generalizations of equations (13), (18) and (20) hold for all diagonals  $k = 0, 1, \dots, K$ , i.e.

$$G(n + 1, n + 1 - k, z) = R_k(n - k, z)G(n, n - k, z) \tag{23}$$

and

$$G(n, n - k, z) = P_k(n - k, z)G(n, n - k + 1, z) \tag{24}$$

for all  $k \leq K$  and  $n \geq k$ . If we prove similar relationships along the  $K + 1$  ‘diagonal’, and given that we checked them explicitly for  $K = 0, K = 1$ , it follows that they hold everywhere. This step is carried out using the equation of motion for  $G(n, n - k, z)$  and using the (already known) ratios indicated in figure 3. This results in

$$C_K(n - K - 1, z)G(n, n - K, z) + G(n - 1, n - K, z) + G(n + 1, n - K, z) = 0, \tag{25}$$

where for any  $n \geq 0$ ,

$$C_K(n, z) = z + \frac{1}{P_K(n, z)R_K(n, z)} + \frac{1}{P_K(n + 1, z)} \tag{26}$$

are known quantities. We now use the same trick as before: we write equation (25) for  $n \rightarrow n + 1$  and use the fact that  $G(n, n - K, z)$  and  $G(n + 1, n + 1 - K, z)$  are related by the known  $R_K(n - K, z)$  ratio. This allows us to find a recurrence relation involving only

$G(n, n - K - 1, z)$ ,  $G(n + 1, n - K, z)$  and  $G(n + 2, n + 1 - K, z)$  values on the  $K + 1$  ‘diagonal’. Asymptotic analysis as  $n \rightarrow \infty$  reveals that equation (22) is indeed obeyed along the  $K + 1$  diagonal, and that for any  $n \geq 0$ ,

$$R_{k+1}(n, z) = \frac{R_k(n + 1, z)}{\frac{C_k(n, z)}{C_k(n+1, z)} [1 + R_{k+1}(n + 1, z)] - R_k(n + 1, z)} \quad (27)$$

with  $R_{k+1}(n \rightarrow \infty, z) = \lambda(z)$ . Finally, using the fact that the last two terms in equation (25) are proportional to each other shows that equation (24) is also obeyed for  $k = K + 1$ , where

$$P_{k+1}(n, z) = -\frac{C_k(n, z)}{1 + R_{k+1}(n, z)}. \quad (28)$$

In the asymptotic limit  $n \rightarrow \infty$ , one can verify that  $P_k(n, z) \rightarrow -2/[1 + \lambda(z)]$ , for all  $k$ .

This completes the proof that indeed we can use continued fractions to calculate all consecutive ratios along each diagonal, as well as the ratios between Green’s functions on neighboring diagonals, starting from the main ones along  $k = 0, k = 1$ . Together with the reference values provided by equation (23), these allow us to calculate any desired  $G(n, m, z)$  without doing any explicit integrals.

These considerations also give the following interesting relationships in the asymptotic limit  $n \rightarrow \infty$ , for any  $m \leq n$ :

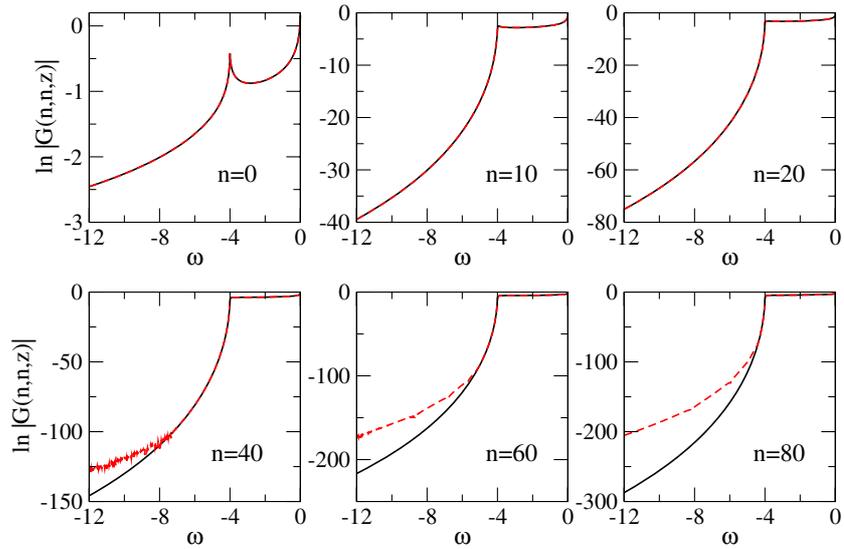
$$G(n + 1, m + 1, z) \approx \lambda(z)G(n, m, z), \quad G(n, m - 1, z) \approx -\frac{z}{2[1 + \lambda(z)]}G(n, m, z). \quad (29)$$

These are rather unusual especially if one tries to derive them directly starting from equation (3). One can also calculate quite easily  $1/n$  corrections. For example, this changes  $\lambda(z) \rightarrow \lambda(z) [1 - \frac{1}{2n+3} + \dots]$  as a better estimate for the value of  $R_0(n, z)$  in the asymptotic limit, etc.

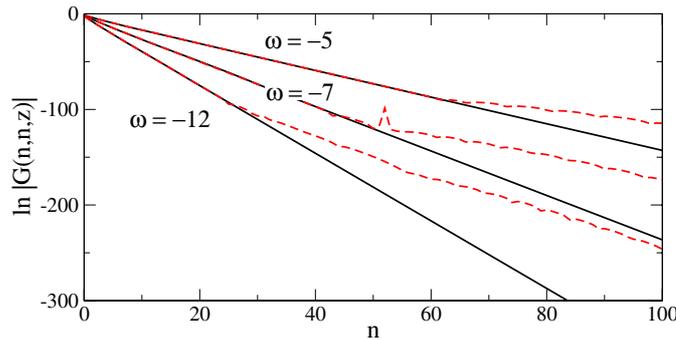
#### 4. Results

In this section, we compare results obtained using the continued fractions method versus those produced by direct numerical integration. We begin, in figure 4, with elements along the main diagonal  $n = m$ . The continued fractions results (black full line) were produced using truncation at  $n_{\max} = 1000$  (this is more than enough to achieve convergence). Note that this means that we obtain *all*  $G(n, n, z)$ ,  $n = 0, n_{\max}$  by doing less than  $14n_{\max}$  elementary multiplications, divisions and additions. This shows that the continued fraction method is much more efficient than direct integration, which certainly requires more than 14 elementary calculations per integral. At small  $n$  and/or energies inside the continuum, the two methods agree well. For larger  $n$  and smaller  $\omega$ , however, the continued fraction method becomes much more accurate, as shown by the fact that it produces a smooth curve, whereas direct numerical integration gives a lot of noise (this is not so obvious for  $n = 60, 80$  because of the scale). Another way to prove that indeed the continued fraction method is more accurate is demonstrated in figure 5, where we plot  $\ln |G(n, n, z)|$  versus  $n$  for several energies outside the continuum. The black lines produced by the continued fraction method show the expected exponential decrease of  $G(n, n, z)$  with the distance  $n$ , whereas the red dashed curves (numerical integration) deviate at large distances—the lower the energy, the shorter the distance at which direct numerical integration starts to produce wrong results.

Similar behavior is found for elements on the second diagonal,  $G(n + 1, n, z)$ , as shown in figure 6, which backs up our claim that the continued-fraction method allows one to calculate very efficiently and accurately any Green’s function along either of these two diagonals.



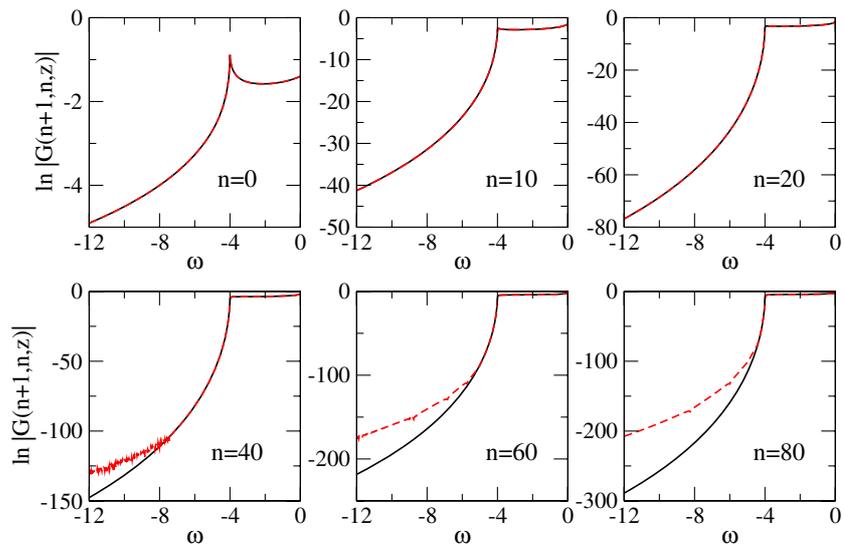
**Figure 4.**  $\ln |G(n, n, z)|$  versus  $\omega$ , for  $n = 0, 10, 20, 40, 60, 80$ , as given by the continued fractions (full black line) and direct integration (red dashed line). In all cases,  $\eta = 0.01$ .



**Figure 5.**  $\ln |G(n, n, z)|$  versus  $n$ , for  $\omega = -5, -7, -12$ , as given by the continued fractions (full black line) and direct integration (red dashed line). In all cases,  $\eta = 0.01$ .

However, for general  $G(n, m, z)$  values, the accuracy of the continued fraction method decreases steadily as  $n - m$  increases, in other words as one moves to diagonals further and further away from the main one. We believe that this is due to errors accumulated as the recurrence relations on diagonals with larger  $k$  values are generated. These errors are linked to the initial values used for  $R_k(n, z)$  at the truncation limit, as demonstrated by the fact that using more accurate values (e.g. including  $1/n$  corrections in the expression of  $\lambda(z)$ ) increases the domain where the method remains very accurate.

Exactly how good or bad the continued-fraction prediction is depends on all parameters  $n, m, z$  in a non-trivial fashion. In all cases where we checked, the predictions were more accurate than those obtained with the Morita scheme, although in some cases both schemes are very wrong. We were unable to find any general criteria to identify ‘safe regions’ where



**Figure 6.**  $\ln |G(n+1, n, z)|$  versus  $\omega$ , for  $n = 0, 10, 20, 40, 60, 80$ , as given by the continued fractions (full black line) and direct integration (red dashed line). In all cases,  $\eta = 0.01$ .

the continued fraction method is always trustworthy, beyond the first two diagonals; while it generally appears that smaller  $n - m$ , more negative  $\omega$  and/or larger  $\eta$  slow the loss of accuracy, one would need to carefully evaluate whether or not to use this method depending on their needs.

To conclude, we have presented here a method which in principle allows one to efficiently evaluate all Green's functions  $G(n, m, z)$  on a square lattice without doing any explicit integrations in terms of continued fractions. In reality, however, we only claim very good accuracy for cases with  $n = m$ ,  $n = m + 1$ . Further than that, one has to be very careful with using this method, but then the same is true with direct numerical integrations which can also fail (see figures 4 and 5) or the Morita scheme.

Given the link between Green's function and hypergeometric functions [2], it is clear that this approach based on using continued fraction to evaluate physical solutions of such recurrence relations can be generalized beyond the problem addressed here. In fact, such recurrence relations are known to appear for many special functions, so this method may turn out to be useful in a much wider context. This possibility will be investigated elsewhere.

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