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# Green's functions on finite lattices and their connection to the infinite lattice limit

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## Abstract

It is shown that the Green's function on a finite lattice in arbitrary space dimension can be obtained from that of an infinite lattice by means of translation operator. Explicit examples are given for one- and two-dimensional lattices.

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## I. INTRODUCTION

Lattice Green's functions (LGF) are widely used in solving discrete (e.g., Schrodinger) equations. In the infinite lattice (or thermodynamic) limit explicit expressions for the LGF in different space dimensions  $d$  are known for a long time [1–4]. The form of the LGF in the direct lattice space ( $X$ ) as obtained by the Fourier transform method is usually given by a  $d$ -fold integral over the reciprocal space ( $Q$ ) that can be further reduced to known functions. This allows, in particular, to obtain the eigenenergy equation in an explicit form too (see, e.g. [3] for an example covering  $d = 1, 2, 3$  of the Heisenberg spin model). An extension of this approach to finite lattices has been proposed in [5]. It is based on an approximation shown to account sufficiently well even for subtle details of the exact solution, known from the Bethe ansatz in the case of a finite spin chain. Control over finite  $N$  (the number of lattice sites along one coordinate) corrections turns to be essential for a proper description of the wave function symmetry and behavior of the eigenenergies. The approach has revealed new classes of excitation modes for lattices in higher dimensions and has allowed to find their connection to those known from Bethe solutions in  $1D$ . The further development of the approach was based on the proof of several exact expressions for the finite lattice sums and the discrete Fourier transform in one dimension [6]. We have recently become aware of the paper [7] where some similar exact formulas have been derived.

In particular, with the discrete Fourier transform (DFT) we reproduce the exact eigenenergy equations known from Bethe ansatz. The latter, however, can not be applied to higher dimensional lattices. In the present paper we generalize the earlier exact formulas to higher dimensions. It turns out that the GF at finite  $N$  can be obtained from that of the infinite lattice under the action of a simple function of the translation operator. This result is tested on the  $d = 1$  case studied earlier and an example for the  $d = 2$  case is also given. Remarkably, the expression for the finite LGF in two dimensions is obtained in a form of a single integral, as the function does not reduce to known ones. Another advantage of the expressions derived in this way, i.e. involving translations with  $N$ , is their efficiency in obtaining exact asymptotic expansions. The approach is rather general and can be applied to different lattice types without limitation on space dimension.

## II. GREEN'S FUNCTION ON A FINITE SQUARE LATTICE

The form of the LGF studied below

$$G_{sq}(X, Y) \equiv \frac{1}{N} \sum_{m=0}^{N-1} \frac{1}{N} \sum_{n=0}^{N-1} \frac{\exp(iQ_x X + iQ_y Y)}{\lambda - \eta \cos(Q_x) - \xi \cos(Q_y)}, \quad (1)$$

$$Q_x = \frac{\Delta_x}{N} + 2\pi \frac{m}{N}; \quad Q_y = \frac{\Delta_y}{N} + 2\pi \frac{n}{N};$$

$$X, Y = 0, 1, \dots, N - 1.$$

is the simplest one and, at the same time, contains the important  $\Delta$ - parameters related to the symmetry of the wave function, as explained in earlier works [5, 6, 8]. For simplicity we also confine the energy parameter  $\lambda$  to the region outside the scattering states,  $\lambda \geq 2$ . Let's consider a simple generalization of the formula expressing (1) in terms of modified Bessel functions [6], [7]

$$G_{sq}(X, Y) = \int_0^\infty dz e^{-\lambda z} \sum_{q=-\infty}^{\infty} \sum_{p=-\infty}^{\infty} I_{pN+X}(z) I_{qN+Y}(z) \exp(-ip\Delta_x - iq\Delta_y), \quad (2)$$

that can be trivially extended to higher dimensions. We then assume  $\eta = \xi$  for simplicity and rescale the  $\lambda$  parameter so that  $\xi = \eta = 1$ . One can easily see that in the thermodynamic limit  $N \rightarrow \infty$  ( $G_{sq}^{TDL}(X, Y)$ ) only the term with  $p = 0$  and  $q = 0$  "survives", e.g., by considering the representation [9]

$$I_n(z) = \int_0^\pi \exp(z \cos y) \cos(ny) \frac{dy}{\pi}, \quad (3)$$

or the formulas for the uniform asymptotic expansion in [9] or Ch. 9 ??,  $I_n(z) \propto \exp(-n \ln(n/C))$ , where  $n, C$  are positive and the fast convergence is illustrated in Fig 9.9.

Eq. (2) then suggests a possibility to act with the "translation operators" like  $\exp(pN \frac{d}{dX})$  upon the  $G_{sq}^{TDL}(X, Y)$  to obtain the full expression at finite  $N$ . It should be taken into account that  $X$  and  $Y$  are defined as above and that due to its symmetry property the modified Bessel function  $I_n(z)$  should actually be written as  $I_{|n|}(z)$ . In this form the action of translation operator on the series is more transparent. Then by splitting the series in two parts we find from (2) that

$$G_{sq}(X, Y) = \int_0^\infty dz e^{-\lambda z} \sum_{q=0}^{\infty} \sum_{p=0}^{\infty} \exp\left(p \left(-i\Delta_x + N \frac{d}{dX}\right)\right) \exp\left(q \left(-i\Delta_y + N \frac{d}{dY}\right)\right) I_{|X|}(z) I_{|Y|}(z)$$

$$\begin{aligned}
 & + \int_0^\infty dz e^{-\lambda z} \sum_{q=0}^\infty \sum_{p=1}^\infty \exp\left(-p\left(-i\Delta_x + N\frac{d}{dX}\right)\right) \exp\left(q\left(-i\Delta_y + N\frac{d}{dY}\right)\right) I_{|X|}(z) I_{|Y|}(z) \\
 & + \int_0^\infty dz e^{-\lambda z} \sum_{p=0}^\infty \sum_{q=1}^\infty \exp\left(p\left(-i\Delta_x + N\frac{d}{dX}\right)\right) \exp\left(-q\left(-i\Delta_y + N\frac{d}{dY}\right)\right) I_{|X|}(z) I_{|Y|}(z) \\
 & + \int_0^\infty dz e^{-\lambda z} \sum_{p=1}^\infty \sum_{q=1}^\infty \exp\left(-p\left(-i\Delta_x + N\frac{d}{dX}\right)\right) \exp\left(-q\left(-i\Delta_y + N\frac{d}{dY}\right)\right) I_{|X|}(z) I_{|Y|}(z).
 \end{aligned}$$

Taking the geometric series of translation operators, we obtain

$$\begin{aligned}
 G_{sq}(X, Y) & = \left[ \frac{1}{1 - \exp\left(-i\Delta_x + N\frac{d}{dX}\right)} + \frac{\exp\left(i\Delta_x - N\frac{d}{dX}\right)}{1 - \exp\left(i\Delta_x - N\frac{d}{dX}\right)} \right] \\
 & \times \left[ \frac{1}{1 - \exp\left(-i\Delta_y + N\frac{d}{dY}\right)} + \frac{\exp\left(i\Delta_y - N\frac{d}{dY}\right)}{1 - \exp\left(i\Delta_y - N\frac{d}{dY}\right)} \right] G_{sq}^{TDL}(|X|, |Y|). \quad (4)
 \end{aligned}$$

Note that the operators in the square brackets do not annihilate each other since they act differently on  $G_{sq}^{TDL}(|X|, |Y|)$ . Expressions (1) and (4) mean that the LGF at finite  $N$  is a linear superposition of the limit LGF translated with multiples of the lattice period. Generalization of Eq. (4) to a lattice in an arbitrary dimension is obvious. With this general representation one can straightforwardly obtain the LGF from the integral representation of LGF in the thermodynamic limit, e.g.

$$G_{sq}^{TDL}(|X|, |Y|) = \int_0^{2\pi} \int_0^{2\pi} \frac{\exp(ip|X|) \exp(iq|Y|)}{\lambda - \cos p - \cos q} \frac{dp dq}{2\pi 2\pi}, \quad (5)$$

using the property

$$f\left(N\frac{d}{dX}\right) \exp(CX) = f(NC) \exp(CX),$$

and that  $|X - N| = N - X$  (where  $f$  is a function and  $C$  a parameter). One can apply it directly to the known expressions of the  $G^{TDL}$  for different lattices.

In the  $d = 1$  case we have

$$G_{1d}^{TDL}(|X|) = \int_0^{2\pi} \frac{\exp(iq|X|)}{\cosh v - \cos q} \frac{dq}{2\pi} = \frac{\exp(-v|X|)}{\sinh v}, \quad (6)$$

where the energy parameter  $\lambda$  has been replaced by  $\cosh v$ . Note that the last equality holds also when the modulus sign on the l.h.s. is omitted. Thus, one finds

$$G_{1d}(X) = \left[ \frac{1}{1 - \exp\left(-i\Delta + N\frac{d}{dX}\right)} + \frac{\exp\left(i\Delta - N\frac{d}{dX}\right)}{1 - \exp\left(i\Delta - N\frac{d}{dX}\right)} \right] \frac{\exp(-v|X|)}{\sinh v}$$

$$= \left[ \frac{\exp(-vX)}{1 - \exp(-i\Delta - Nv)} + \frac{\exp(i\Delta + (X - N)v)}{1 - \exp(i\Delta - Nv)} \right] \frac{1}{\sinh v}, \quad (7)$$

i.e. the result obtained earlier [6]. For the sake of comparison to higher dimensional lattice we also give the result of applying the operator to the first equality in (6) and leading to the same result:

$$\int_0^{2\pi} \frac{\exp(iqX)}{\cosh v - \cos q} \times \frac{1}{1 - \exp(-i\Delta + iqN)} \frac{dq}{2\pi} + \int_0^{2\pi} \frac{\exp(-iqX)}{\cosh v - \cos q} \times \frac{\exp(i\Delta + iqN)}{1 - \exp(i\Delta + iqN)} \frac{dq}{2\pi}.$$

However in the case of square lattice such a direct application of translation operators to  $G_{sq}^{TDL}(|X|, |Y|)$  does not reduce to a known function. Generally,  $G_{2D}^{TDL}$  is a double hypergeometric Appel function [2], that can be reduced to elliptic integrals in more simple cases (as the one considered in the present paper). Then we can use the approach defined by (4) and discussed below. An equivalent way would be to substitute in (2) the well known integral representations of Bessel function involving exponentials [9] as (3) and

$$I_n(at) I_m(at) = \int_0^{2\pi} \frac{dy}{2\pi} I_{n+m}(2at \cos y) \exp(-i(n-m)y),$$

to finally reduce  $G_{sq}(X, Y)$  to a single integral.

In analogy with the  $d = 1$  case, according to (4) and (5), we have ( $\gamma = 2/\lambda$ )

$$\int_0^{2\pi} \frac{dp}{2\pi} \int_0^{2\pi} \frac{dq}{2\pi} \frac{1}{2 \cos \lambda - \cos p - \cos q} \times \left[ \frac{\exp(ipX)}{1 - \exp(-i\Delta_x + ipN)} + \frac{\exp(-ipX) \exp(i\Delta_x + ipN)}{1 - \exp(i\Delta_x + ipN)} \right] \times \left[ \frac{\exp(iqY)}{1 - \exp(-i\Delta_y + iqN)} + \frac{\exp(-iqY) \exp(i\Delta_y + iqN)}{1 - \exp(i\Delta_y + iqN)} \right]. \quad (8)$$

The product of the first terms in square brackets is then transformed as below

$$\sum_{m=0}^{\infty} \sum_{n=0}^{\infty} \int_0^{2\pi} \frac{dQ}{2\pi} \exp(iQ(X + mN - Y - nN) - im\Delta_x - in\Delta_y) \times \int_0^{2\pi} \frac{dP}{2\pi} \times \frac{\exp(iP(X + mN + Y + nN))}{\cos \lambda - \cos P \cos Q},$$

and after taking the last integration, we obtain the expression

$$\gamma \int_0^{2\pi} \frac{d\phi}{2\pi} \frac{\exp(f(\phi)(X + Y))}{\sqrt{1 - (\gamma \cos \phi)^2}} \exp(i\phi(Y - X)) \times \sum_0 \sum_0 \exp(i\phi(nN - mN)) \exp(f(\phi)(mN + nN)),$$

where

$$f(\phi) \equiv \ln \left( \frac{\gamma \cos \phi}{1 + \sqrt{1 - (\gamma \cos \phi)^2}} \right).$$

The final result can be presented in the following form

$$G_{sq}(X, Y) = \frac{1}{N} \sum_{m=0}^{N-1} \frac{1}{N} \sum_{n=0}^{N-1} \frac{\exp(iQ_x X + iQ_y Y)}{\lambda - \cos(Q_x) - \cos(Q_y)} = \frac{\gamma}{4\pi} \int_0^{2\pi} \frac{d\phi}{\sqrt{1 - (\gamma \cos \phi)^2}} \times \quad (9)$$

$$\left( \frac{\exp(Xf^-)}{(1 - \exp(-i\Delta_x + Nf^-))} + \frac{\exp(i\Delta_x + (N-X)f^-)}{(1 - \exp(i\Delta_x + Nf^-))} \right) \times \left( \frac{\exp(Yf^+)}{(1 - \exp(-i\Delta_y + Nf^+))} + \frac{\exp(i\Delta_y + (N-Y)f^+)}{(1 - \exp(i\Delta_y + Nf^+))} \right),$$

where

$$f^+ \equiv f(\phi) + i\phi; \quad f^- \equiv f(\phi) - i\phi.$$

The structure of this exact expression is surprisingly simple and indicates the possibility of extension to other lattices. In particular, (9) contains the periodic symmetry of the LGF represented by the transformation  $X \rightarrow (N - X)$  and  $Y \rightarrow (N - Y)$ . For  $X, Y \ll N$  and  $\gamma \neq 1$  we find in the thermodynamic limit,  $N \rightarrow \infty$ :

$$G_{sq}^{TDL}(X, Y) = \frac{\gamma}{4\pi} \int_0^{2\pi} \frac{\exp(i\phi(Y - X))}{\sqrt{1 - (\gamma \cos \phi)^2}} \left( \frac{\gamma \cos \phi}{1 + \sqrt{1 - (\gamma \cos \phi)^2}} \right)^{X+Y} d\phi. \quad (10)$$

Eq. (10), the "byproduct" of (9), gives at the same time a convenient integral representation for the hypergeometric function  ${}_4F_3$  - the explicit form of the  $G_{sq}^{TDL}(X, Y)$  found in [2], that arises in various other contexts, see, e.g. [11]. In particular, for  $X = Y = 0$  we find the known result containing the elliptic integral of the first kind

$$G_{sq}^{TDL}(0, 0) = \frac{2}{\pi\lambda} K \left( \frac{2}{\lambda} \right) \quad (11)$$

Another important observation is that in the  $N \rightarrow \infty$  limit the symmetry related information contained in the  $\Delta$ -parameters seems to be lost. However, recalling our earlier results, the slow  $N$ -convergence of the "correction" terms in the vicinity of the critical condition  $\gamma = 1$  proves that the symmetry of the corresponding solutions of the Schrodinger equation on a



two-dimensional lattice is retained even in the thermodynamic limit. Away from the critical condition the symmetry of the wave function shows up in its large scale properties, i.e. when  $X/N, Y/N$  are not small.

In conclusion, the main result of the paper is the derivation of new exact expressions for the Green's function on a finite two-dimensional lattice. It is shown that these expressions are the result of applying a simple function of translation operator to the Green function of the infinite lattice. The derivation outlines the way for generalizations to other lattice types or dispersion relations other than simple cosine and different space dimensions. The exact result (9) does not correspond to a known special function, but reduces to such ones in particular cases. The structure of the exact expression is appropriate for the development of asymptotic expansions. The latter are straightforward away from the critical parameter region and can be found by standard methods in the vicinity of critical values of parameters. The integral formulas can be continued to the region of the energy parameter corresponding to the "scattered states", i.e.  $\lambda < 2$ . These further developments will be considered in other publications.

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