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Lattice Green Function for a Free Massive Boson

KOMA Yoshiaki *

Abstract: The Green functions characterize interaction properties between particles in quantum field theories. We evaluate the Green functions for a massive scalar boson defined on a three-dimensional Euclidean lattice numerically, and investigate the lattice effect by comparison with the continuum Green function. We again find a characteristic difference at very short distances quantified approximately by an exponential function as in the massless case.

Key Words: Green function, Propagator, Lattice formulation

1. Introduction

Formulating a quantum field theory on a discretized spacetime, which we call the lattice formulation in short, regularizes the continuum theory that has an infinite number of degrees of freedom with a finite number of them. In this formulation, field variables of the theory are treated as a finite number of site or link variables, and then, it is possible to solve the field equations by using a kind of finite difference methods or to compute the partition function of the theory by using the Monte-Carlo method. A weak point, however, may be that the numerical results always suffer from systematic errors due to finite cutoff and finite volume even if one obtains precise results. This is because one cannot perform computation practically in infinite volume with infinitesimally small lattice spacing. Therefore, it is important to control the lattice artifacts in the numerical results.

The evaluation of the Green functions defined on the lattice, which we call the lattice Green functions, may provide us with some hints for controlling the lattice effect. The Green functions play the role of propagators in quantum field theories, which contain information on the interaction properties between particles. For instance, when a massless boson, such as the photon in quantum electrodynamics, carries a continuum momentum p_μ, its propagator in the momentum representation is given by $1/p^2$, which corresponds to the well-known Coulombic potential $\propto 1/r$ in the coordinate representation. On the lattice, however, the momentum is discretized and its range is also restricted due to finiteness of the lattice spacing and the volume, which should affect the behavior of the Green function. Thus, the comparison of the lattice results with the continuum one will help to expose the lattice artifacts.

Previously, we investigated the lattice Green function for the massless boson defined on a three-dimensional Euclidean lattice numerically and compared the results with the continuum one [1]. We then found a characteristic difference at very short distances, which is quantified approximately by an exponential function. As we mentioned, the remnant of such an exponential behavior may cause a problem when a theory that can generate a mass dynamically is analyzed, since the effect of the mass usually appears as an exponential function.

In the present report, we extend our previous work to the case that a propagating particle has a finite mass m. More specifically, we investigate the lattice Green functions for a free massive scalar boson in three-dimensional Euclidean space. In the continuum theory, it is known that the particle obeys the Klein-Gordon equation, so that the propagator with the momentum p_μ is given by $1/(p^2+m^2)$ and the Fourier transformation leads to the Yukawa potential $\propto e^{-mr}/r$. We shall compare the lattice results with this continuum behavior.

2. The lattice Green functions

In the continuum theory, the Green function $G(x;m)$ for a massive scalar boson is defined by the relation

$$(-\Delta + m^2)G(x;m) = \delta(x) \,, \tag{1}$$

where Δ denotes the Laplacian and $\delta(x)$ the Dirac delta function. The solution of Eq. (1) in the n-dimensional space can be obtained by performing the Fourier transformation of the Green function in the

*Division of Liberal Arts

momentum representation $1/(p^2+m^2)$ as

$$G(x;m) = \int_{-\infty}^{\infty} \frac{d^n p}{(2\pi)^n} \frac{e^{ipx}}{p^2+m^2} \ , \tag{2}$$

where $p^2 = \sum_{\mu=1}^n p_\mu p_\mu$, $ipx = i\sum_{\mu=1}^n p_\mu x_\mu$. By using the integral formula $F^{-1} = \int_0^\infty d\alpha e^{-\alpha F}$, the Fourier transformation is carried out as [2]

$$\begin{aligned} G(x;m) &= \int_0^\infty d\alpha \int \frac{d^n p}{(2\pi)^n} e^{ipx} e^{-\alpha(p^2+m^2)} \\ &= \int_0^\infty d\alpha\, e^{-\alpha m^2} \prod_{\mu=1}^n \int_{-\infty}^{\infty} \frac{dp_\mu}{2\pi} e^{-\alpha(p_\mu - \frac{ix_\mu}{2\alpha})^2 - \frac{x_\mu^2}{4\alpha}} \\ &= \int_0^\infty d\alpha\, e^{-\alpha m^2} \left(\frac{1}{2\pi}\right)^n \left(\frac{\pi}{\alpha}\right)^{\frac{n}{2}} e^{-\frac{x^2}{4\alpha}} \\ &= \frac{1}{(2\pi)^{\frac{n}{2}}} \left(\frac{m}{r}\right)^{\frac{n}{2}-1} K_{\frac{n}{2}-1}(mr) \ , \end{aligned} \tag{3}$$

where the final expression is based on the integral formula of the modified Bessel function of the second kind

$$K_\nu(z) = \frac{1}{2}\left(\frac{z}{2}\right)^\nu \int_0^\infty dt\, e^{-t-\frac{z^2}{4t}} t^{-\nu-1} \quad (\nu \in \mathbb{R}) \ . \tag{4}$$

Therefore, for the $n=3$ case the Green function is reduced to the well-known Yukawa potential

$$G(x;m) = \frac{1}{(2\pi)^{\frac{3}{2}}} \left(\frac{m}{r}\right)^{\frac{1}{2}} K_{\frac{1}{2}}(mr) = \frac{e^{-mr}}{4\pi r} \ , \tag{5}$$

where $K_{1/2}(z) = \sqrt{\pi/(2z)}\, e^{-z}$ is used.

On the lattice in *infinite* volume, the Green function $G_\infty(x;m)$ should satisfy

$$(-\Delta + m^2) G_\infty(x;m) = \delta_{x0} \ , \tag{6}$$

where $\Delta = \sum_{\mu=1}^n \nabla_\mu^* \nabla_\mu$ denotes the lattice Laplacian, which is a combination of the forward and backward differences, so that $\Delta f(x) = \sum_{\mu=1}^n [f(x+\hat{\mu}) + f(x-\hat{\mu}) - 2f(x)]$, and δ_{x0} is the Kronecker delta, satisfying $\delta_{x0} = 1$ for $x = 0$ and $\delta_{x0} = 0$ for $x \neq 0$. The momentum carried by a particle is defined by $\hat{p}_\mu = 2\sin(p_\mu/2)$, where $p_\mu \in [-\pi, \pi]$. The lattice spacing is set to be one throughout this report. Note that due to hypercubic symmetry, the lattice Green functions near the origin satisfy a relation

$$(2n+m^2) G_\infty(0;m) - 2n G_\infty(\hat{\mu};m) = 1 \ . \tag{7}$$

The Fourier transformation is carried out similarly as

$$\begin{aligned} G_\infty(x;m) &= \int_{-\pi}^{\pi} \frac{d^n p}{(2\pi)^n} \frac{e^{ipx}}{\hat{p}^2+m^2} \\ &= \int_{-\pi}^{\pi} \frac{d^n p}{(2\pi)^n} \frac{e^{ipx}}{4\sum_{\mu=1}^n \sin^2(p_\mu/2) + m^2} \\ &= \int_0^\infty d\alpha\, e^{-(2n+m^2)\alpha} \\ &\quad \times \prod_{\mu=1}^n \int_{-\pi}^{\pi} \frac{dp_\mu}{2\pi} e^{2\alpha\cos p_\mu + ip_\mu x_\mu} \\ &= \int_0^\infty d\alpha\, e^{-(2n+m^2)\alpha} \prod_{\mu=1}^n I_{x_\mu}(2\alpha) \ , \end{aligned} \tag{8}$$

where the final expression is based on the integral formula of the modified Bessel function of the first kind

$$I_\nu(z) = \frac{1}{\pi}\int_0^\pi d\theta e^{z\cos\theta} \cos\nu\theta \quad (\nu \in \mathbb{Z}) \ . \tag{9}$$

Since the integration over α cannot be carried out analytically, one may resort to numerical integration. The convergence property of this integration, however, is expected to be quite slow for large α, due to the behavior of the modified Bessel function $I_\nu(2\alpha) \sim \sqrt{1/(4\pi\alpha)} e^{2\alpha}$ for large α. In fact, the integrand will be of $O(\alpha^{-n/2})$ and this asymptotic behavior indicates that it may be difficult to obtain precise numerical values for lower dimensions $n \leq 3$ except for the large mass cases.

For the massless case with $n = 4, 3, 2$, this problem is solved [3–5]. If one applies to a similar method, the procedure is modified as in Ref. [6] with a relation

$$(\nabla_\mu^* + \nabla_\mu) G_\infty(x;m) = x_\mu \int_{-\pi}^{\pi} \frac{d^n p}{(2\pi)^n} e^{ipx} \ln(\hat{p}^2 + m^2) \ . \tag{10}$$

Inserting Eq. (10) into Eq. (6) for $x \neq 0$, one obtains a recursion relation

$$\begin{aligned} &G_\infty(x+\hat{\mu};m) = G_\infty(x-\hat{\mu};m) \\ &+ \frac{2x_\mu}{\rho} \sum_{\nu=1}^n [(1+\frac{m^2}{2n}) G_\infty(x;m) - G_\infty(x-\hat{\nu};m)] \end{aligned} \tag{11}$$

with $\rho = \sum_{\mu=1}^n x_\mu$ for $\rho \neq 0$. We do not proceed further this method in this report, but examine if the numerical result satisfies the relation in Eq. (6).

On the lattice in *finite* volume of the size $V = \prod_{\mu=1}^n L_\mu$, where periodic boundary conditions are imposed in all μ directions, the Green function $G_L(x;m)$ should satisfy the same relation as in Eq. (6), but the

Table 1: The lattice Green functions for $m = 0.50$ in infinite volume and in finite volume of $V = 24^3$.

r	$G_\infty(r;m)$	$G_\infty(r;m) - G_\infty(0;m)$	$G_L(r;m)$	$G_L(r;m) - G_L(0;m)$
0	$2.111547903170267\times10^{-1}$	0	$2.111549304663567\times10^{-1}$	0
1	$5.328623991356951\times10^{-2}$	$-1.578685504034572\times10^{-1}$	$5.328638590245488\times10^{-2}$	$-1.578685445639018\times10^{-1}$
2	$1.708696890778575\times10^{-2}$	$-1.940678214092410\times10^{-1}$	$1.708713461306398\times10^{-2}$	$-1.940677958532927\times10^{-1}$
3	$6.642001737189745\times10^{-3}$	$-2.045127885798370\times10^{-1}$	$6.642208288145088\times10^{-3}$	$-2.045127221782116\times10^{-1}$
4	$2.934166508491701\times10^{-3}$	$-2.082206238085350\times10^{-1}$	$2.934449547507940\times10^{-3}$	$-2.082204809188487\times10^{-1}$
5	$1.402515601993884\times10^{-3}$	$-2.097522747150329\times10^{-1}$	$1.402937062890787\times10^{-3}$	$-2.097519934034659\times10^{-1}$
6	$7.042904660635528\times10^{-4}$	$-2.104504998509632\times10^{-1}$	$7.049587589070812\times10^{-4}$	$-2.104499717074496\times10^{-1}$
7	$3.654127104022456\times10^{-4}$	$-2.107893776066245\times10^{-1}$	$3.665181733324653\times10^{-4}$	$-2.107884122930242\times10^{-1}$
8	$1.940082167762876\times10^{-4}$	$-2.109607821002504\times10^{-1}$	$1.958861987254369\times10^{-4}$	$-2.109590442676312\times10^{-1}$
9	$1.047841774237187\times10^{-4}$	$-2.110500061396030\times10^{-1}$	$1.080283405645461\times10^{-4}$	$-2.110469021257921\times10^{-1}$
10	$5.735009830886571\times10^{-5}$	$-2.110974402187179\times10^{-1}$	$6.301773058981373\times10^{-5}$	$-2.110919127357669\times10^{-1}$
11	$3.172329212786405\times10^{-5}$	$-2.111230670248989\times10^{-1}$	$4.171101085926890\times10^{-5}$	$-2.111132194554974\times10^{-1}$
12	$1.770079724664004\times10^{-5}$	$-2.111370895197801\times10^{-1}$	$3.544003416786985\times10^{-5}$	$-2.111194904321888\times10^{-1}$

momentum is modified to $p_\mu(k) = 2\pi l_\mu(k)/L_\mu$ with integers $l_\mu(k) = 0, 1, 2, ..., L_\mu - 1$, reflecting the periodicity $G_L(x;m) = G_L(x + L_\mu\hat{\mu};m)$. The Fourier transformation is then given by summation instead of integration as

$$G_L(x;m) = \frac{1}{V}\sum_k \frac{e^{i\sum_{\mu=1}^n \frac{2\pi l_\mu(k)}{L_\mu}x_\mu}}{4\sum_{\mu=1}^n \sin^2(\frac{\pi l_\mu(k)}{L_\mu}) + m^2}. \quad (12)$$

In contrast to the massless case, there is no need to remove the zero momentum mode. The summation over all momenta is easily achieved by using a FFT algorithm. When the lattice volume is isotropic such as $L_\mu = L$ for all μ directions, the relation like in Eq. (7) holds for G_L due to hypercubic symmetry.

3. Numerical results

We shall present numerical results in three dimensions. Since our aim is to reveal the lattice effects in the lattice Green function, we first focus on the difference of the lattice Green functions in infinite and finite volumes, where the mass is set to be $m = 0.50$ as an example.

In Table 1, we show the numerical values of Eq. (8) evaluated by using Wolfram Mathematica, and of Eq. (12) obtained by using a FFT algorithm of SciPy on the $V = 24^3$ lattice, both along the on-axis $x = (r, 0, 0)$. An interesting observation is that $G_\infty(r;m)$ and $G_L(r;m)$ are quite similar with each other. If one looks at the numerical values in Table 1 carefully, however, one may notice that there is a small

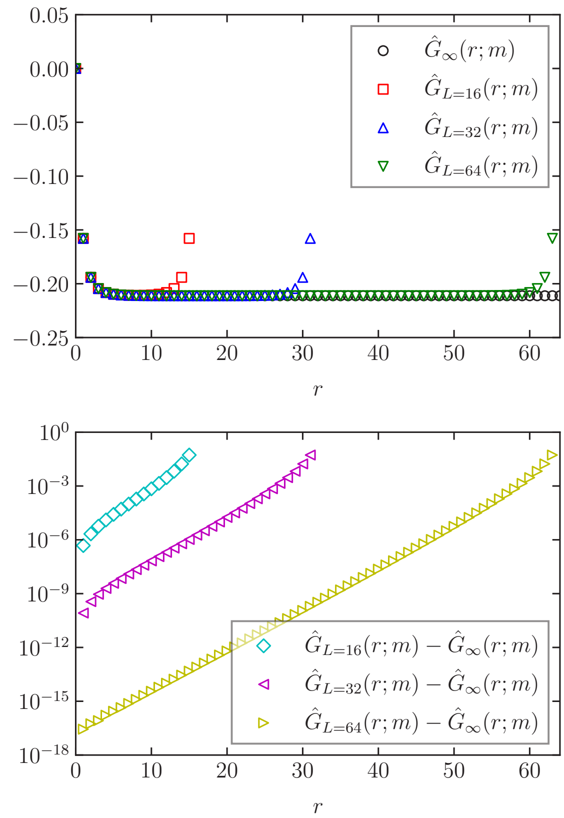

Fig. 1: The normalized lattice Green function in infinite volume $\hat{G}_\infty(r;m)$ and in finite volume $\hat{G}_L(r;m)$(upper), and the difference $\hat{G}_L(r;m) - \hat{G}_\infty(r;m)$ (lower).

discrepancy, which seems to increase gradually with the distance r. The reason will be obvious by plotting the numerical values of various lattice volumes for all range of $r \in [0, L]$ as shown in Fig. 1. The systematic increase of the difference just reflects the periodicity

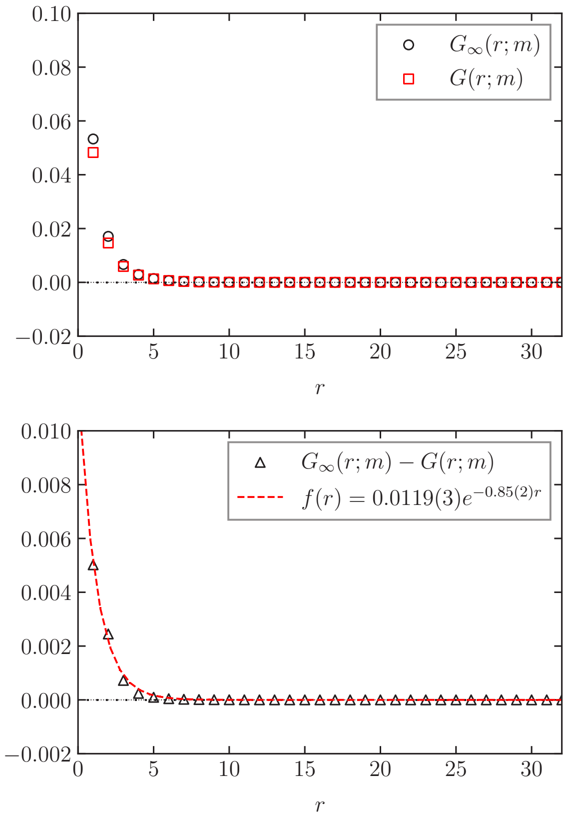

Fig. 2: The lattice Green function in infinite volume $G_\infty(r;m)$ and the continuum Green function $G(r;m) = e^{-mr}/(4\pi r)$ (upper), and the difference $G_\infty(r;m) - G(r;m)$ (lower).

of the lattice in finite volume. This means that it can easily be controlled by taking a reasonably large lattice volume. Thus, in order to investigate the lattice effect based on comparison with the continuum Green function, either type of the lattice Green functions can be used (of course, the lattice volume should appropriately be large when the finite volume one is used). Note for the massless case that the coincidence of the lattice Green function in infinite and finite volumes can be observed only for the normalized one [1].

We then compare the lattice Green function in infinite volume $G_\infty(r;m)$ and the continuum Green function $G(r;m) = e^{-mr}/(4\pi r)$ in Fig. 2. In the continuum case, the Green function at the origin is divergent due to the $1/r$ behavior, so that we pay attention to the range for $r \geq 1$. We find that both lattice and continuum Green functions show a similar behavior with an exponential suppression for r, and only at very short distances for $r \leq 5$ there appears a characteristic difference by about ten percent. A chi-square fitting analysis for the difference $G_\infty(r;m) - G(r;m)$ indicates that this approximately obeys an exponential function

$$f(r) = 0.0119(3)e^{-0.85(2)r} . \tag{13}$$

What is remarkable is that the functional form and the fitting parameters are quite similar to that in the massless case [1]. We note that if we assume the functional form of the $G_\infty(r;m)$ as of the continuum one, $p_1 e^{-p_2 r}/r$, and perform chi-square fitting analyses, the parameter corresponding to the mass, p_2, can be appropriate only when we neglect the data at short distances, such that $p_2 = 0.5009(4)$ for $6 \leq r \leq 20$, while $p_2 = 0.535(2)$ for $2 \leq r \leq 20$.

4. Summary

We have investigated the lattice Green function for a scalar massive boson numerically both in finite and infinite volumes in three-dimensional Euclidean space. Our results again exhibit a characteristic difference from the continuum Green function at very short distances for $r \leq 5$, which is quantified by using an exponential function as in the massless case. Thus, one should be careful to use the continuum Green function to extract physical parameters such as a mass from the lattice result when only the short distance data is available. The origin of the exponential difference need to be investigated further.

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