Scaling Hypothesis of Spatial Search on Fractal Lattice Using Quantum Walk

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We investigate a quantum spatial search problem on fractal lattices, such as Sierpinski carpets and Menger sponges. In earlier numerical studies of the Sierpinski gasket, the Sierpinski tetrahedron, and the Sierpinski carpet, conjectures have been proposed for the scaling of a quantum spatial search problem finding a specific target, which is given in terms of the characteristic quantities of a fractal geometry. We find that our simulation results for extended Sierpinski carpets and Menger sponges support the conjecture for the optimal number of the oracle calls, where the exponent is given by $1/2$ for $d_s > 2$ and the inverse of the spectral dimension $d_s$ for $d_s < 2$. We also propose a scaling hypothesis for the effective number of the oracle calls defined by the ratio of the optimal number of oracle calls to a square root of the maximum finding probability. The form of the scaling hypothesis for extended Sierpinski carpets is very similar but slightly different from the earlier conjecture for the Sierpinski gasket, the Sierpinski tetrahedron, and the conventional Sierpinski carpet.

I. INTRODUCTION

The complex network is ubiquitous in many real-world systems, including the World-Wide-Web, social and biological networks, such as the actors network, protein-protein interaction network, and cellular network [1]. Contrary to conventional wisdom that the complex networks are not the self-similar due to the “small-world” property, the renormalization technique has revealed that the structure of the complex network is indeed self-similar [1]. The efficient database search on such networks is an important issue, and one of the efficient schemes is to apply the spatial search using quantum walk, which has been applied to a random network, the so-called Erdős–Renyi random graphs [2]. In this respect, studying the quantum spatial search on fractal geometries is relevant to practical application to real-world systems composed of complex networks with self-similarity, and yet there naturally arises a fundamental question; what kind of scaling law is behind the quantum spatial search on self-similar networks. The fractal lattice, such as the Sierpinski gasket, Sierpinski carpet, or Menger sponge, is one of the simplest but most fundamental structures to investigate this problem.

A spatial search problem is a kind of database search to find a marked item from a given $N$-site graph. A quantum search algorithm [3] using quantum walk provides faster performance than classical search algorithm [4]. This so-called Grover’s algorithm, as well as the Shor’s algorithm, are well-known algorithms based on quantum mechanics [5]. Nowadays the quantum walk can be experimentally implemented in various systems, such as an optical lattice [6], an ion trap [7], and photonic systems [8–11].

The idea of the Grover’s algorithm is to amplify the probability finding a target point [3]. It is achieved by repeatedly applying a quantum oracle operator and then applying the Grover’s diffusion operator. The quantum oracle operator changes the sign of the probability amplitude of the target site, and the Grover’s diffusion operator provides the inversion about the mean. Since it obeys a unitary evolution, the dynamics of the probability finding a specific target is periodic as a function of the number of oracle calls. A helpful intuitive picture for understanding the quantum spatial search is a Schrödinger dynamics on a lattice with a single attractive potential at the target site [12].

After the Grover’s paper [3], the quantum search has been intensively and extensively studied [4, 12–28]. One of the main issues is to understand the scaling relation between the optimal number of oracle calls $Q$ and the number of sites $N$. The scaling behavior varies strongly depending on the spatial dimension of the graph. For $d = 1$, the scaling law is $Q = O(N)$, which means that the efficiency is equivalent to that of classical search [13, 17]. For $d > 2$, the scaling law is $Q = O(\sqrt{N})$ in a hypercubic lattice for the continuous-time or discrete-time algorithm [14–17], which is consistent with the original Grover’s search [3]. On the other hand, the two-dimensional system is critical, which gives the scaling law in the form $Q = O(\sqrt{N \ln^s N})$ [13–18]. Indeed, for $d = 2$, the relations $Q = O(\sqrt{N \ln^{3/2} N})$ [14] and $O(\sqrt{N \ln N})$ [15, 16] are reported. In $d = 2$, the faster search algorithm, which gives $Q = O(\sqrt{N \ln N})$, is also proposed by Tulsi, which employs an ancilla qubit [17, 18].

From these results, Patel and Raghunathan argued that the scaling law for spatial search in $d$-dimension obeys [17]

$$Q \geq \max\{dN^{1/d}, \pi \sqrt{N}/4\},$$

(1)

except for $d = 2$, where emerges the logarithmic slowing down analogous to critical phenomena in statistical mechanics [20]. Based on this formula, they posed the following questions: does the relation (1) hold in the non-integer dimensional system? If so, what is an appropriate dimension $d$ appearing in (1)? In general, the fractal system is characterized by following three kinds of the dimension; the Euclidean dimension, the fractal dimension, and the spectral dimension; definitions of these
dimensions will be given in the next section.

Using the Sierpinski gasket and Sierpinski tetrahedron, Patel and Raghunathan numerically found that $d$ is given by the spectral dimension $d_s$, but not the fractal dimension; they proposed the conjecture of the scaling law [22]

$$Q \geq \max\{N^{1/d_s}, \pi \sqrt{N}/4\}. \quad (2)$$

In order to check the validity of this conjecture, Tamegai and two of the authors recently investigated the scaling law (2) by using the Sierpinski carpet [27], which has the fractal and spectral dimensions different from the Sierpinski gasket and Sierpinski tetrahedron. They found that the scaling law is consistently given by the spectral dimension rather than by the fractal dimension in the case of the Sierpinski carpet.

Furthermore, they proposed a novel scaling hypothesis about the effective number of the oracle calls, defined by $Q/\sqrt{P_{\text{max}}}$ in the fractal lattice, where $P_{\text{max}}$ is the maximum probability at the marked site. They found that the scaling exponent $\gamma$, given by $Q/\sqrt{P_{\text{max}}} = O(N^\gamma)$, is expressed by a combination of characteristic quantities of a fractal structure [27]:

$$\gamma = \frac{d_s}{d_E - 1} + d_f - s, \quad (3)$$

which involves the Euclidean dimension $d_E$, the fractal dimension $d_f$, the spectral dimension $d_s$, and the scaling factor $s$. This relation holds very well within the margin of error in the Sierpinski carpet [27]. Furthermore, the same relation was shown to hold excellently also in the Sierpinski gasket and Sierpinski tetrahedron by using the numerical data reported by Patel and Raghunathan [22].

In this study, based on the studies of Refs. [22, 27], we further investigate the scaling hypotheses proposed in Refs. [22, 27] in various kinds of fractal lattices: extended Sierpinski carpets, a conventional Menger sponge, and extended Menger sponges. In the extended Sierpinski carpets, the scaling hypothesis for the optimal number of oracle calls (2) holds very well. In the Menger sponge case, where the Euclidean and fractal dimensions are greater than 2, i.e., $d_{E,f} > 2$, the scaling exponent gets saturates at the value close to 1/2. In the extended Sierpinski carpets, although the scaling hypothesis (3) does not exactly hold, we find a variant of the scaling law very similar to (3), which fits our numerical data very well.

This paper is organized as follows. Section II introduces quantities characterizing a fractal geometry, such as the Euclidean dimension, fractal dimension, spectral dimension, and scaling factor. Section III describes the spatial search algorithm with the discrete-time quantum walk. Section IV provides numerical simulation results, and discuss the scaling hypothesis. Finally, we conclude our results in Sec. V.

II. FRACTAL GEOMETRY

Fractal geometry is ubiquitous in nature showing self-similar patterns [30]. In this section, we briefly introduce quantities characterizing a fractal geometry, such as the Euclidean dimension, fractal dimension, spectral dimension as well as the scaling factor, which appear in scaling hypotheses discussed in this paper.
For a self-similar pattern created by eliminating small pieces from the structure according to a certain rule, the relation $M(s) = s^{d_E}$ no longer holds. In that case, one extends the definition of the dimension. If $M(s) = s^{d_s}$ holds for arbitrary $s$ in the self-similar pattern, the scaling exponent $d_s$ is called the fractal dimension. In Menger sponge (Fig. 1), for example, one has $d_t = \ln 20/\ln 3 = 2.55\cdots$.

The spectral dimension $d_s$ is related to a dynamical property of a classical random walk. One of the definitions is to relate $d_s$ to a scaling behavior of the return probability through $P_c(x_0,t) \propto t^{-d_s/2}$, where a random walker starts from a specific site $x_0$ at $t = 0$ [31, 32]. The Sierpinski gasket has an explicit form of the spectral dimension, given by $d_s = 2 \ln (d_E + 1)/\ln (d_E + 3)$. However, since no analytic forms of the spectral dimension

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are known for Sierpinski carpets and Menger sponges at present, we numerically calculate the spectral dimensions from the scaling analysis of the return probability.

For evaluating the spectral dimension, we consider the following discrete-time random walk. First, we randomly choose a single site $x_0$ on the fractal lattice, where the walker starts the classical random walk. At each time step, the walker moves 1 unit in the randomly chosen direction (for example, in the case of Sierpinski carpet, we chose right, left, down, or up randomly with probability 1/4 each). If the nearest neighbor site does not exist in the chosen direction, the walker stays on the present site. Repeating this process, the diffusive behavior of the random walk on the fractal lattice can be analyzed. The return probability is estimated by the relation $P_t(x_0, t) = N(x_0, t) / N_{\text{trial}}$, where $N(x_0, t)$ is the number of the events where the particle returns to the starting point $x_0$ at a time $t$, and $N_{\text{trial}}$ is the number of trials of the discrete-time random walk. Here, we take $N_{\text{trial}} = 1,000,000$ in this study to evaluate the spectral dimension. We have determined the spectral dimension from the scaling fit as shown in Fig. 2.

Table I summarizes characteristic quantities of fractal lattices discussed in the present paper. For Sierpinski carpets and Menger sponges, we use symbols SC($s, s'$) and MS($s, s'$), respectively, in this paper. Here, $s$ is a scaling factor that gives the number of sites on each side in the smallest unit. We then create empty sites, the number of which is $s'$ on each side also in the smallest unit (Fig. 3). For the spectral dimension $d_s$, our results are consistent with the earlier prediction for the upper and lower bounds within the margin of error [29] (See Table I).

III. SPATIAL SEARCH USING FLIP-FLOP WALK

In this study, we use a spatial search algorithm with flip-flop walk [22, 27]. A state $|\Psi\rangle$ obeys a discrete time evolution performed by an oracle operator $\hat{R}$ and a flip-flop walk operator $\hat{W}$, given by

$$|\Psi(t)\rangle = (\hat{W}\hat{R})^t |\Psi(t = 0)\rangle. \quad (5)$$

The state $|\psi(t)\rangle \equiv \sum_{x, l} a_{x,l}(t) |x\rangle \otimes |l\rangle$ is defined in the Hilbert space $\mathcal{H}_{\text{search}} \equiv \mathcal{H}_N \otimes \mathcal{H}_K$, where $|x\rangle \in \mathcal{H}_N$ is associated with the position degree of freedom, and $|l\rangle \in \mathcal{H}_K$ is associated with the internal degree of freedom with the link vector $l$ that orients a nearest neighbor site.

The oracle operator is given by $\hat{R} = \hat{R}_N \otimes I_K$ with $\hat{R}_N = I_N - 2|x_0\rangle \langle x_0|$, where $I_N$ and $I_K$ are the identity operators in $\mathcal{H}_N$ and $\mathcal{H}_K$, respectively, and $x_0$ is the position of a target. The operator $\hat{R}$ plays a role of an attractive potential that enhances the finding probability at the marked vertex. The flip-flop walk operator $\hat{W}$ is composed of a Grover diffusion operator $\hat{G}$ and a flip-flop shift operator $\hat{S}$, i.e., $\hat{W} = \hat{S}\hat{G}$. The Grover diffusion operator [3] evolves the probability amplitude as follows:

$$a_{x,l} \xrightarrow{\hat{G}} \frac{2}{k} \sum_{l'} a_{x,l'} - a_{x,l}. \quad (6)$$

We employ $k = 4$ for a Sierpinski carpet and $k = 6$ for a Menger sponge. The flip-flop shift operator $\hat{S}$ propagates a probability amplitude along its link direction with the link vector flipped:

$$|x\rangle \otimes |l\rangle \xrightarrow{\hat{S}} |x+1\rangle \otimes |-l\rangle. \quad (7)$$

When we consider a fractal lattice, there are missing sites (for example, the gray area in Fig.3). In this case, we employ the following [27]:

$$|x\rangle \otimes |l\rangle \xrightarrow{\hat{S}} |x\rangle \otimes |l\rangle. \quad (8)$$

As an initial state, we use the uniform superposition state:

$$|\psi(t = 0)\rangle = \frac{1}{\sqrt{N_K}} \sum_{x} \sum_{l} |x\rangle \otimes |l\rangle. \quad (9)$$

The probability $P(x, t)$ at a time step $t$ on a site $x$ is given by

$$P(x, t) = \sum_{l} |\langle x| \otimes \langle l| |\Psi(t)\rangle|^2 = \sum_{l} |a_{x,l}(t)|^2. \quad (10)$$

In the numerical simulation, we follow the formalism of discrete-time quantum walk based on Eq. (5)–(10). The time evolution of the probability amplitude $a_{x,l}(t)$ is updated by following the rules of the oracle operator $\hat{R}$, and the flip-flop walk operator $\hat{W}$, where a set of operators $\hat{W}\hat{R}$ gives the discrete-time evolution $|\Psi(t + 1)\rangle = \hat{W}\hat{R}|\Psi(t)\rangle$. The initial probability amplitude is prepared as $a_{x,l}(t = 0) = 1/\sqrt{N_K}$, which corresponds to the uniform superposition state in Eq. (9).

IV. SIMULATION RESULTS

Figure 4 shows a typical example of the time evolution of the probability on the Sierpinski carpet SC(3, 1). The probability is concentrated at the target site and then diffuses, repeatedly (Sierpinski carpets in Fig. 5 (a) and Menger sponges in Fig. 6 (a)).

In order to analyze the scaling law, we perform numerical simulation about 100, 000-1, 000, 000 steps for Sierpinski carpets, and 5, 000-100, 000 steps for Menger sponges. The optimal number of an oracle call $Q$, which is a characteristic period of the probability at a target site $x_0$, is evaluated from a frequency giving the maximum intensity of the Fourier transformation of $P(t, x_0)$. We also determine the mean value of the maximum probability $P_{\text{max}}$. Here, a data set of $P(t, x_0)$ is chronologically grouped with a period $Q$, and then the maximum
values are evaluated in each group. By using this data set of maximum values, we calculate the mean value of the maximum probability \( P_{\text{max}} \). The optimal number of oracle call \( Q \) and the mean value of maximum probability \( P_{\text{max}} \) are shown as functions of the number of sites \( N \) in Figs. 5 (b) and (c) for Sierpinski carpets, and in Figs. 6 (b) and (c) for Menger sponges. We analyze the scaling law by supposing the relation \( Q = O(N^\beta) \) and \( P_{\text{max}} = O(N^{-\alpha}) \). The exponents \( \alpha \) and \( \beta \) obtained from the numerical data are summarized in Table II.

Patel and Raghunathan proposed the scaling hypothesis (2), given in the form \( Q \geq \max\{N^{1/d_s}, \pi \sqrt{N/4}\} \) [22]. In order to check this conjecture, we plot the scaling exponent \( \beta \), given by \( Q \propto N^\beta \), as a function of the spec-
rection is expected to emerge from data shown in Fig. 5 (b) and 6 (b) for the Sierpinski carpet (SC) and the Menger sponge (MS), respectively. It also includes the data of the Sierpinski carpet (SC), Sierpinski gasket (SG) and Sierpinski tetrahedron (ST) reported in Refs. [22, 27] for non-integer dimensions as well as the data of hypercubic lattices (Lattice) in Refs. [13–17] for integer dimensions. The exponent follows the relation $\beta = 1/d_s$ for $d_s < 2$, and saturates at $\beta = 1/2$ for $d_s > 2$. For the spectral dimension close to the critical dimension $d_s \simeq 2$, the exponent $\beta$ does not follow the relation $\beta = 1/d_s = 1/2$, which may suggest the necessity of the logarithmic correction.

To study the scaling law in more detail, we summarize values $\beta$ and $1/d_s$ in Table II for Sierpinski carpets and Menger sponges. In the Sierpinski carpets, where $d_s < d_t < d_E = 2$, we find that the scaling hypothesis $\beta = 1/d_s$ holds well. In the Menger sponges, where $2 \leq d_s < d_t < d_E = 3$, the relation $\beta \simeq 1/d_s$ does not hold. In this case, we find $\beta \simeq 0.5$, which reproduces $Q = O(\sqrt{N})$ as in the scaling law (2). In particular, in the case where the spectral dimension $d_s$ is sufficiently greater than 2, such as the case of MS(3,1), the relation $\beta = 1/2$ is well reproduced, which is consistent with the hypercubic lattice case in $d > 2$ [14–17]. In the case where $d_s \simeq 2$, the scaling hypothesis (2) is not reproduced (see Fig. 7 and Table II). In $d_s = 2$, the logarithmic correction is expected to emerge $Q \propto \sqrt[N]{\ln^\epsilon N}$ [13–18]. We analyzed the exponent of this logarithm close to $d_s = 2$, and obtained the following fitting results: $\epsilon = 0.62(9)$ for MS(4,2), $\epsilon = 0.689(5)$ for MS(5,3), and $\epsilon = 0.84(3)$ for MS(6,4).

Patel and Raghunathan proposed another scaling relation [22]

$$\alpha = 2\beta - 1, \quad (11)$$

in the context of the Tulsi’s amplification algorithm for the success probability. In Table II, we find the relation $\alpha - 2\beta + 1 \simeq 0$ seems to hold. In particular, we find that the scaling relation (11) holds within the margin of error for the Menger sponges with $2 < d_t < d_E = 3$.

Finally, we investigate the scaling of the effective number of oracle calls $Q/\sqrt{P_{\text{max}}} = O(N^{\gamma})$. The exponents $\gamma' = \gamma''$ are given in Eqs. (13) and (14), respectively.

$$\begin{array}{|c|c|c|c|c|c|}
\hline
\text{Lattice} & \text{SC} & \text{ST} & \text{MS} \\
\hline
\text{L} & 0.64(1) & 0.645(8) & 0.317(4) & 0.007(1) & 0.325(4) \\
\text{SC} & 0.60(1) & 0.606(7) & 0.275(7) & 0.04(2) \\
\text{ST} & 0.55(2) & 0.64(1) & 0.320(3) & 0.04(2) \\
\text{MS} & 0.50(2) & 0.666(8) & 0.38(1) & 0.08(4) \\
\hline
\end{array}$$

TABLE III. Scaling of the effective number of oracle calls $Q/\sqrt{P_{\text{max}}} = O(N^{\gamma})$. The exponents $\gamma'$ and $\gamma''$ are given in Eqs. (13) and (14), respectively.
responds to the case where \( s' = 1 \), the scaling hypothesis is given by

\[
\gamma = \frac{d_s}{d_E - 1} + d_f - s, \tag{13}
\]

which holds within an error as shown in Ref. [27]. In the extended Sierpinski carpet SC(2 + \( s' \), \( s' \)) for \( s' > 1 \), we find that the hypothesis (13) does not hold (Table III), which suggests that we may need another scaling law. Here, we propose a hypothesis for \( s' > 1 \) analogous to (13), given in the form

\[
\gamma = \frac{1}{2} \left( \frac{d_s}{d_E - 1} + d_f - \frac{s}{s'} \right). \tag{14}
\]

As shown in Table III, the scaling hypothesis (14) is reproduced within an error for \( s' > 1 \) in the extended Sierpinski carpets, where \( d_s < d_f < d_E = 2 \). In the conventional Menger sponge MS(3, 1) for \( d_s = 2.55(6) \), we find that the relation (14) approximately holds. However, in the case of the extended Menger sponges MS(2 + \( s' \), \( s' \)) with \( s' > 1 \) for \( d_s \approx 2 \), we find that both scaling conjectures (13) and (14) do not hold. Indeed, close to \( d_s = 2 \), the system may be in the critical regime.

In short, there may be the scaling law for the effective number of oracle calls in the Sierpinski carpet for \( d_s < 2 \), which is given by quantities characterizing a fractal geometry, such as the Euclidean dimension, the fractal dimension, the spectral dimension and the scaling factor. For the conventional Sierpinski carpet with \( s' = 1 \), the scaling relation (13) holds reasonably well. For the extended Sierpinski carpet with \( s' > 1 \), the scaling relation (14) holds well within the margin of error. For the Menger sponges, on the other hand, the scaling relation (11) holds well within the margin of error.

An important issue for future study is to prove the conjectures (2), (13), and (14). One of an interesting approach may be to employ idea of the renormalization [24, 25]. Since the relations (13) and (14) are reproduced very well, we naturally expect that there should be a beautiful mathematical structure behind the quantum spatial search on a fractal geometry. We further need to explore the scaling law for a non-integer dimension close to \( d_s = 2 \), where the logarithmic correction may be expected. Finally, the reason of the appearance of the factor 1/2 in (14), compared with (13), must be clarified. One of the possible origin of the factor 1/2 might be given by \( 1/(s - s') \) for \( s' > 1 \), although we have studied only the case for \( s - s' = 2 \) in this paper.

In recent experiments, the quantum walk can be performed in an optical lattice [6], an ion trap [7], and photonic systems [8–11]. Furthermore, single electron in real space is accessible in Sierpinski gasket fabricated on Cu(111) by using scanning tunneling microscopy and spectroscopy [33]. With these developments, we hope that the quantum spatial search on the fractal lattice will become accessible in near future to confirm the scaling behavior of the finding probability at a specific target. Indeed, the spatial search may be emulated by the continuous-time Schrödinger dynamics on the lattice with a single attractive potential site [12, 19]. For example, suppose that an optical lattice with a fractal geometry is prepared. Then, trap a single atom in it for making the uniform superposition state in the fractal lattice. It may be more preferable to use a macroscopic matter wave of the Bose–Einstein condensate (BEC). By analyzing the time-evolution of the finding probability or the density profile of the BEC with use of the single atom addressing technique [34, 35], the scaling behavior depending on the topological structure of the lattice may be studied as in the present paper. Dynamical properties at a specific local site may be governed by the global structure of the fractal lattice, such as the dimensions, and the scaling factor. We hope that the present study further promotes interdisciplinary study of complex networks, mathematics and quantum mechanics on the fractal geometry.

V. CONCLUSIONS

Many real-world systems, such as the World-Wide-Web, social and biological networks, exhibits the complex network structure. Developing an efficient search algorithm on such complex networks is an important issue, and one of the efficient ways is to apply the spatial search by quantum walk. An interesting point is that these complex networks may have the self-similarity in spite of the “small-world” property. In addition to the important practical problem of applying quantum spatial search to each real-world system composed of complex networks, there naturally arises the fundamental question, namely, what kind of scaling law is behind the quantum spatial search on self-similar networks, such as fractal lattices.

We investigated the spatial search using quantum walk on various kinds of fractal lattices, such as Sierpinski carpets and Menger sponges. We first studied the conjecture by Patel and Raghunathan proposed for the Sierpinski gasket and tetrahedron, and corroborated their conjecture for other fractal lattices, where the exponent for the optional number of oracle calls with respect to the number of sites is given by the inverse of the spectral dimension \( d_s \) for \( d_s < 2 \), and approaches 1/2 for \( d_s \) being far from 2. For \( d_s \approx 2 \), the deviation from their conjecture emerges, which supports the fact that the two-dimensional system is critical and the logarithmic correction may be needed. We also studied the relation between the exponent for the optimal number of oracle calls and the exponent for the mean value of the maximum probability at a specific target.

Finally, we proposed the scaling conjecture of the effective number of oracle calls, which is given by characteristic quantities of the fractal geometry, such as the Euclidean dimension, fractal dimension, spectral dimension, as well as the scaling factor. The relation for the extended Sierpinski carpets proposed in this paper is similar but slightly different from the relation proposed by Tamegai and two of the authors for the Sierpinski gasket, Sier-
pinski tetrahedron, and conventional Sierpinski carpet. Nevertheless, it may be indeed a fact that the quantum spatial search on the fractal lattice is surprisingly subject to the combination of the characteristic quantities of the fractal geometry. It is an open question why the scaling law of the effective number of oracle calls is given by such combination of the dimensions and the scaling factor. Mathematical proofs of these scaling relations have not been also provided yet, and are left for a future study.

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