Ultradiffusion and biased ultradiffusion on a regular fractal

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By an exact real-space renormalization-group approach, we investigate ultradiffusion with a hierarchical pattern of hopping rates defined on the regular Vicsek fractal. Anomalous long-time behavior of the autocorrelation function of ultradiffusion is observed. It is found that the transition from anomalous to normal diffusion occurs in the general n-dimensional case, and the transition point is independent of dimension. In the presence of bias, we find another unusual transition that leaves hopping particles trapped in some areas in contrast to the diffusive state for which the average square distance $\langle R^2(t)\rangle \sim \infty$ for $t \to \infty$. This transition is essentially different from the one for biased ultradiffusion of the one-dimensional multiple-furcation hierarchical system.

It is known that hierarchical structures occur in several physical systems from molecular diffusion on complex macromolecules[1] to spin glasses[2] and computing structures.[3] Therefore, considerable interest has been recently focused on hierarchical systems to study diffusion dynamics,[4,5] the Schrödinger equation,[6,7] and the Ising problem,[8] etc. Huberman and Kerszberg[4] proposed an ultradiffusion model in hierarchical structures to explain the anomalous relaxation that has been observed in wide range of physical phenomena such as spin glasses and random-field Ising magnets.[9] They found an anomalous decay process, i.e., the transition in dynamics from normal to anomalous diffusion. This is termed the one-dimensional ultradiffusion model because of the characteristic ultrametric topology and its anomalous decay process.[5,10] Normally, the ultradiffusion model consists of the hopping of a particle in a hierarchical array of barriers. For this system the time-dependent probability distribution satisfies a master equation of the form

$$\frac{d}{dt}P_n(t)=\sum_{m\{\mathrm{NN}\}} w_{m,n}[P_m(t)-P_n(t)] , \qquad (1)$$

where $P_n(t)$ is the probability of finding the particle in the nth cell at time t, $w_{m,n}$ is the probability per unit of time that the particle hops from the nth cell to the mth, and $w_{m,n}=w_{n,m}=w_i$. The sum is taken over nearest neighbors (NN's).

Here we present the study of the ultradiffusion problem defined on the regular Vicsek fractal.[11,12] Its hierarchical barriers are same as those of Riera's study[13] of relaxation on Sierpinski gaskets. This fractal was introduced by Vicsek as a model embodying the essential feature of diffusion-limited aggregation (DLA).[14] Subsequent studies concerning this fractal structure have been made of the Ising problem,[15] percolation,[12] and the random-walk[16,17] problem. In our ultradiffusion model, the hierarchical structure of the barriers could be determined from its fractal nature. When the particle hops between two cells at points connecting first-stage generators, we denote its hopping rate w_0. When the particle crosses the points connecting second-stage generators, its hopping rate is w_2 and so on. So energy barriers are labeled corresponding to the connecting points of the two cells (see Fig. 1). The diffusion process we consider is that where the particle hops from a cell n to its nearest neighbors m through the barrier i with a hopping probability w_i defined above. As shown in Fig. 1(a), the hopping rate per unit time between two cells connecting two i-stage generators is denoted by w_i, and the arrangement of w_i is hierarchical. Note we have three types of cells, for example, A,B,C, with different neighbors or different diffusion circumstances. When we perform a Laplace transformation on master equation (1) of this system, we should treat the three types of cells separately with different transform frequencies $\lambda_1,\lambda_2,\lambda_3$. The following equations are the Laplace-transformed equations for the three different types of cells:

$$\begin{aligned}
\lambda_1\tilde{P}_C &= \delta_{C,0}+w_0(\tilde{P}_{C_1}-\tilde{P}_C)+w_0(\tilde{P}_{C_2}-\tilde{P}_C)\\
&\quad +w_0(\tilde{P}_{C_3}-\tilde{P}_C)+w_0(\tilde{P}_{C_4}-\tilde{P}_C) ,\\
\lambda_2\tilde{P}_B &= w_0(\tilde{P}_{B_2}-\tilde{P}_B)+w_i(\tilde{P}_Y-\tilde{P}_B) ,\\
\lambda_3\tilde{P}_A &= w_0(\tilde{P}_{A_2}-\tilde{P}_A) ,
\end{aligned} \qquad (2)$$

where $\tilde{P}$ is the Laplace transform of $P(t)$. The term $\delta_{m,0}$ specifies the initial condition that the particle is supposed to start its random walk at cell 0.

The equations for all cells are listed in Eq. (2). Those transformed equations will be treated with the real-space renormalization-group (RSRG) technique to determine the long-time behavior of the autocorrelation function

$P_0(t)$. The RG approach amounts to a dynamics decimation of (2) carried out in such a way as to leave its basic structure invariant. The hierarchical structure of barriers still exists, but the system is spatially scaled to Fig. 1(b) by a factor $b=3$. The RG procedure will decimate (referring to Fig. 1) all cells except $A,B,C,D,E,\ldots$ and change the set of equations. For example, for cell B, $\lambda_2'\tilde{P}'_B = w_0(\tilde{P}'_C - \tilde{P}'_B) + w'_{i-1}(\tilde{P}'_Y - \tilde{P}'_B)$. So the surviving $\tilde{P}_n$ still satisfy a similar equation with respect to the original one, but with rescaled parameters: frequencies λ_i and hopping probability w_i. The rescaled parameters are given by the following recursion relations:

$$w_i' = \frac{w_0+3w_1}{w_1} w_{i+1} \quad (i \geq 1) , \tag{3a}$$

$$\tilde{P}' = \frac{w_1}{w_0+3w_1} \tilde{P} , \tag{3b}$$

and

$$\begin{bmatrix} \lambda_1' \\ \lambda_2' \\ \lambda_3' \end{bmatrix} = \begin{bmatrix} \dfrac{w_0+7w_1}{w_1} & \dfrac{4(w_0+4w_1)}{2_1} & 8 \\ \dfrac{w_0+2w_1}{w_1} & \dfrac{2w_0+5w_1}{w_1} & \dfrac{2w_0+4w_1}{w_1} \\ \dfrac{w_0+2w_1}{w_1} & \dfrac{w_0+2w_1}{w_1} & \dfrac{3w_0+7w_1}{w_1} \end{bmatrix} \begin{bmatrix} \lambda_1 \\ \lambda_2 \\ \lambda_3 \end{bmatrix} . \tag{3c}$$

In deriving relations of Eqs. (3), we have used the condition $w_0' = w_0$ to fix the time scale. The above relations have been written by abandoning the terms of $O(\lambda)$ in the limit $\lambda \to 0$ in order to study the leading behavior at long time ($t \to \infty$). It is also assumed that cell $c=0$, at which diffusion starts, survives decimation in such a way that the inhomogeneous equation for $\tilde{P}'_0$ remains of the same form as the one for $\tilde{P}_0$.

The solution for the fixed points leads to a whole line of fixed points $\{w_i^*\}$:

$$w_i^* = w_1^* \left[\frac{w_1^*}{w_0^* + 3w_1^*} \right]^{i-1} , \tag{4a}$$

$$w_1^* = \frac{w_0 R}{1-3R} . \tag{4b}$$

Equation (4b) is derived from (4a):

$$\frac{w_{i+1}^*}{w_i^*} = \frac{w_1^*}{w_0^* + 3w_0^*} (=R) .$$

The value of w_1^* can range from $0 \to \infty$. The fixed point $w_1^* = 0$ describes the situation of trapping due to the infinite barriers. The fixed point $w_1^* \sim \infty$ corresponds to the case of zero-height barriers, where we expect normal diffusion to take place. One may expect that the autocorrelation function, which has a probability $P_0(t)$ of coming back to cell 0 at time t, has a scaling behavior of the form $P_0(t) \sim t^{-x/2}$ when $t \to \infty$. The exponent x can be obtained by the inverse Laplace transformation[13] and scaling argument. It is straightforward to derive: $x = 2d_f \ln b / \ln \chi_{\max}$. d_f is fractal dimension. $\chi_{\max}$ is the maximum eigenvalue of the transform matrix of characteristic frequencies λ_i. From (3c) it is easy to find

$$\chi_{\max} = \frac{5(3w_1^* + w_0)}{w_1^*} . \tag{5}$$

The exponent x is as follows:

$$x = \frac{2 \ln 5}{\ln[5(w_0 + 3w_1^*)/w_1^*]} . \tag{6}$$

Referring to the calculation of density of states by Teitel and Domany,[18] one may derive how the diffusion constant $D(R)$ goes to zero and how the anomalous diffusion region approaches to normal diffusion as $R \to \frac{1}{3}$. Note that $x = 2\ln 5 / \ln 15$ is the case of normal diffusion on this fractal structure. So $R_c = \frac{1}{3}$ is the critical point where the transition from normal ($R \geq \frac{1}{3}$) to anomalous diffusion ($R < \frac{1}{3}$) takes place.

The above results can be generalized to arbitrary dimensions. One may consider a similar diffusion problem by taking into account the geometrical symmetries of n-dimensional Vicsek fractal. The recursion relations similar to Eqs. (3) can be obtained. We find that the transform matrix of frequencies is related to dimension n, and the corresponding exponent x may be derived easily as

$$x = \frac{2 \ln(2^n + 1)}{\ln[(2^n+1)(w_0 + 3w_1^*)/w_1^*]} . \tag{7}$$

In the limit $w_1^* \to \infty$, it is reduced to

$$x = \frac{2 \ln(2^n+1)}{\ln[3(2^n+1)]} ,$$

which should be the case of normal diffusion on the n-dimensional Vicsek fractal. When $d=1$ its hierarchical structure reduces to the one-dimensional (1D) bifurcate hierarchical barriers in Zheng, Lin, and Tao,[19] and our results coincide exactly with theirs. For the general n-dimensional case, the recursion relation still gives $w_1^* = Rw_0/(1-3R)$, which breaks down at $R_c = \frac{1}{3}$. So we may conclude that the transition from ultradiffusion to normal diffusion occurs at $R_c = \frac{1}{3}$. This shows that the anomalous decay process which was indicated to occur on 1D hierarchical structure by Huberman and Kerszberg still exists in the general n-dimensional Vicsek fractal. An interesting result is that the transition point R_c is independent of dimension. We have also found that the scaling behaviors of w_i and $\tilde{P}$ remain the same for different dimensions.

We turn to the ultradiffusion in the presence of external field since previous studies[19,20] had found a transition at $\eta = w_0$ from a power-law to (hierarchy-dependent) exponential decay of $P_0(t)$ for biased ultradiffusion. Now we apply an external field denoted by η to this system that biases the diffusion in a specific direction. We will find that biased ultradiffusion on this fractal may have more attractive behavior than we had expected. Its master equation in the presence of external force with the same hierarchical barriers is as follows:

$$\lambda_i \tilde{P}_n = \sum_{m\{\text{NN}\}} w_{m,n}(\tilde{P}_m - \tilde{P}_n) + \sum_{m\{\text{NN}\}} \sigma_{m,n}\eta(\tilde{P}_m - \tilde{P}_n) . \tag{8}$$

One may find that this model seems reasonable only when $\eta \le \min\{w_i\}$ from the above equation, and the case of $\eta > \min\{w_i\}$ may be considered afterwards. $\sigma_{m,n} \in \{-1, 0 \text{ or } 1\}$ depend on the positions of m,n and the direction of bias. The direction of bias η is important to our result. We chose a bias in the **x** direction which is identical to **y** because of the symmetry of the fractal. Performing the Laplace transform on the master equation also with the three types of characteristic frequencies $\lambda_1, \lambda_2, \lambda_3$ and following the same renormalization procedure, the recursion relations of w_i, $\tilde{P}$, η, and $\{\lambda_i\}$ can be obtained. The RG decimation (referring to Fig. 1) yields to a series of equations of the same form as the original one (8), but with rescaled parameters with following recursion relations:

$$w_i' = \Omega w_{i+1} \quad (i \ge 1) , \tag{9a}$$

$$\tilde{P}' = \tilde{P}/\Omega , \tag{9b}$$

$$\eta' = \Omega \eta , \tag{9c}$$

$$\begin{bmatrix} \lambda_1' \\ \lambda_2' \\ \lambda_3' \end{bmatrix} = [\mathbf{M}] \begin{bmatrix} \lambda_1 \\ \lambda_2 \\ \lambda_3 \end{bmatrix} , \tag{9d}$$

where

$$\Omega = \frac{w_0(w_0^3 + 3w_0^2 w_1 + 3w_0\eta^2 + w_1\eta^2)}{w_0^3 w_1 + 3w_0^2\eta^2 + 3w_0 w_1 \eta^2 + \eta^4} ,$$

$$[\mathbf{M}] = \begin{bmatrix} \alpha & \beta & \dfrac{w_0^2+\eta^2}{w_0^2-\eta^2}\gamma \\ \theta & \delta+\Omega & \dfrac{2(\omega_0^2+\eta^2)}{w_0^2-\eta^2}\theta \\ \theta & \delta & \Omega + \dfrac{2(w_0^2+\eta^2)}{w_0^2-\eta^2}\theta \end{bmatrix} ,$$

with

$$\alpha = (w_0^4 + 7w_0^3 w_1 + 11 w_0^2 \eta^2 + 5 w_0 w_1 \eta^2)/\Delta ,$$

$$\beta = 4(w_0^4 + 4w_0^3 w_1 + 3w_0^2\eta^2)/\Delta ,$$

$$\gamma = 8(w_0^3 w_1 + w_0 w_1 \eta^2 + 2 w_0^2 \eta^2)/\Delta ,$$

$$\delta = (w_0^4 + 2w_0^3 w_1 + 3w_0^2\eta^2 + 2w_0 w_1 \eta^2)/\Delta ,$$

$$\theta = w_0^2(w_0^2 + 2w_0 w_1 + \eta^2)/\Delta ,$$

$$\Delta = w_0^3 w_1 + 3w_0^2\eta^2 + 3w_0 w_1\eta^2 + \eta^4 .$$

The scaling relation of η has three fixed points $\eta^* = 0, \pm w_0$. The first fixed point $\eta_1^* = 0$ corresponds to the case of unbiased ultradiffusion, and the second one $\eta_2^* = w_0$ leads a strange long-time behavior of the autocorrelation function. $\eta_1^* = 0$ is the unstable fixed point, but $\eta_2^* = w_0$ is a stable one. Another solution is $\eta^* = -w_0$, which is merely the negative direction of bias. So the phase diagram is very simple. Indeed, it is straightforward to check that, starting at any value of η except $\eta = 0$, the system scales, according to (9c), into the fixed points $\eta^* = \pm w_0$. We write down the leading item of the maximum eigenvalue $\chi_{\max}$ of the transform matrix of $\{\lambda_i\}$ near the fixed point $\eta_2^* \to w_0$:

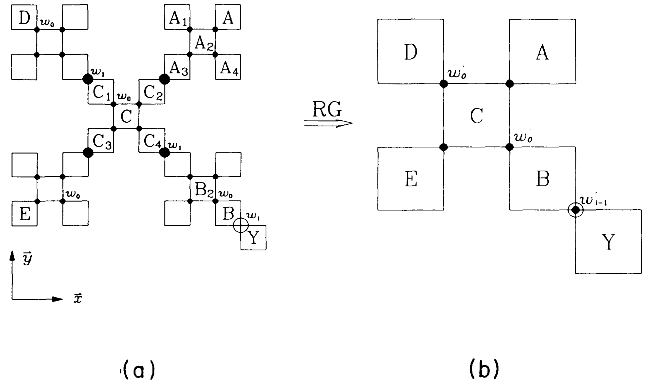

FIG. 1. (a) Hierarchical barriers on the Vicsek fractal. Hopping rates w_i over energy barriers between cells are marked with connecting points. The cells denoted by subscripts are decimated. (b) Fractal structure after RG decimation.

$$\chi_{\max} \overset{\eta^* \to w_0}{\Longrightarrow} \frac{4w_0(w_0 + w_1^*)}{w_1^*(w_0 - \eta^*)} \sim \infty .$$

Therefore, the exponent x is computed as

$$x = \frac{2d_f \ln b}{\ln \chi_{\max}} \xrightarrow{\eta^* \to w_0} 0 . \tag{10}$$

With the autocorrelation function $P_0(t) \sim t^{-x/2}$, we find that $P_0(t)$ tends to a finite value, not infinity. This indicates that, in the presence of bias, the particle will be trapped in some cells. We also observe that the average square distance $R^2(t)$, which has the asymptotic behavior $R^2(t) = \sum_i P_i(t) i^2 \sim t^x$ for $t \to \infty$, will become finite near η_2^*. When $\eta > w_0$ we may expect that the system will be in a frozen trapping state according to the flow diagram near fixed points. We conclude that a phase transition from an ultradiffusion to a trapping state has taken place when the bias is applied. Also, this transition has the following properties: (1) The transition is related to the direction of the bias η. The directions of **x** and **y** are symmetrical. Our calculation shows that there is no such transition when η is in the direction of $\mathbf{n} = \mathbf{x} + \mathbf{y}$. (2) Only when the bias direction is diagonal, $\mathbf{n} = \mathbf{x} + \mathbf{y}$, could one observe the transition from power-law to exponential decay[20] of $P_0(t)$ for this hierarchical structure. In other directions, it could not be found because it is erased entirely by the existence of the trapping transition. (3) The system enters into a trapping state irrespective of the parameter R. The trapping state is different from the one of $w_0 = 0$ in which the particle is trapped by infinite barriers.

In deducing these conclusions, one may make some remarks on the supposition of the three different characteristic frequencies λ_i. The RG decimation procedure illustrates that the maximum eigenvalue does not depend on the supposition that the λ_i overlap. Conversely, the different neighbors of each site, for example, at the quadrafurcate points and bifurcate points, must be considered because of their different scaling behaviors. This is the same as the scaling argument of lattice vibration dynamics. We could suppose different lattice masses instead of the monatomic case, but the maximum eigenvalue still remains the same at low frequencies $\lambda \rightarrow 0$.

In summary, we have used the RSRG technique to demonstrate that the transition from anomalous to normal diffusion occurs on the ultradiffusion model of the general n-dimensional Vicsek fractal. The anomalous-diffusion exponents for the autocorrelation function $P_0(t)$ are obtained. Referring to results for other ultradiffusion structures, we conclude that the exponent x is nonuniversal, but depends on system parameters, the arrangement of barriers, and dimensionality. We find that a phase transition, which results from the bias, takes place from an ultradiffusion to a trapping state. Our research is directly motivated by recent Monte Carlo studies[21] of relaxation on diffusion-limited aggregation. We hope that such a transition of a particle subject to a force falling into a trapping state could be expected to occur in some structures of DLA.

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