Universality in Random-Walk Models with Birth and Death

Carl M. Bender
Department of Physics, Washington University, St. Louis, Missouri 63130

Stefan Boettcher
Department of Physics, Brookhaven National Laboratory, Upton, New York 11973

Peter N. Meisinger
Department of Physics, Washington University, St. Louis, Missouri 63130
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Models of random walks are considered in which walkers are born at one site and die at all other sites. Steady-state distributions of walkers exhibit dimensionally dependent critical behavior as a function of the birth rate. Exact analytical results for a hyperspherical lattice yield a second-order phase transition with a nontrivial critical exponent for all positive dimensions $D \neq 2, 4$. Numerical studies of hypercubic and fractal lattices indicate that these exact results are universal. This work elucidates the adsorption transition of polymers at curved interfaces.

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To study the dynamics governing dissipative systems having an interface [1], we consider random-walk models in which walkers are born at one site and die at all other sites. On the basis of numerical studies, we believe that the critical behavior exhibited by such models is universal. Thus, we define a spherically symmetric random-walk model for which we can obtain exact analytical results. This model uses a *one-dimensional* radial lattice. While this lattice is not translationally invariant, it is suitable for studying spherically symmetric boundary-value problems in any dimension $D > 0$ because it faithfully represents the spatial entropy of the system. This lattice enables us to calculate the adsorption transition of a polymer growing near an attractive boundary [2].

A random walk on a lattice is described by $C_{\mathbf{n},t;\mathbf{m}}$, the probability that a random walker who begins at site $\mathbf{m}$ at $t = 0$ will be at site $\mathbf{n}$ at time t; $C_{\mathbf{n},t;\mathbf{m}}$ satisfies

$$C_{\mathbf{n},t;\mathbf{m}} = \sum_{\{\sigma\}_\mathbf{n}} P(\sigma \to \mathbf{n}) C_{\sigma,t-1;\mathbf{m}} , \qquad (1)$$

where $\{\sigma\}_\mathbf{n}$ is the set of sites σ adjacent to $\mathbf{n}$ and $P(\mathbf{n} \to \mathbf{n}')$ is the probability that a walker at site $\mathbf{n}$ will go to $\mathbf{n}'$ in one step. The initial condition is $C_{\mathbf{n},0;\mathbf{m}} = \delta_{\mathbf{n},\mathbf{m}}$. Local conservation of probability is expressed by $\sum_{\{\sigma\}_\mathbf{n}} P(\mathbf{n} \to \sigma) = 1$ (all $\mathbf{n}$).

We now generalize (1) to allow random walkers to be born with birth rate a at site $\mathbf{0}$ and to die at all other sites with uniform death rate z. Walkers are born or die at a site in proportion to the number of walkers at that site; a and z are the constants of proportionality. (Note that a is a birth rate if $a > 1$; if $a < 1$, it is really a death rate. A similar interpretation holds for z.) Because birth and death rates apply to populations rather than individuals, we study the distribution $G_{\mathbf{n},t}$, which represents the number of random walkers at site $\mathbf{n}$ at time t; $G_{\mathbf{n},t}$ obeys the same recursion relation as $C_{\mathbf{n},t;\mathbf{m}}$ except for factors of a and z:

$$G_{\mathbf{n},t} = \begin{cases} z \sum_{\{\sigma\}_\mathbf{n}} P(\sigma \to \mathbf{n}) G_{\sigma,t-1} & (\mathbf{n} \notin \{\sigma\}_\mathbf{0}), \\ aP(\mathbf{0} \to \mathbf{n}) G_{\mathbf{0},t-1} + z \sum_{\{\sigma \neq \mathbf{0}\}_\mathbf{n}} P(\sigma \to \mathbf{n}) G_{\sigma,t-1} & (\mathbf{n} \notin \{\sigma\}_\mathbf{0}). \end{cases} \qquad (2)$$

Note that $G_{\mathbf{n},t} \geq 0$ for all $\mathbf{n}$ and t. We seek steady-state solutions of Eq. (2); the existence of such solutions imposes a relationship between a and z. All normalizable initial distributions $G_{\mathbf{n},0}$ lead to the same large-t steady-state behavior because a random walk is a diffusive (dissipative) process; the details of $G_{\mathbf{n},0}$ are irretrievably lost as time evolves.

To define a random walk on a D-dimensional spherically symmetric lattice [3], let site n be the region between two concentric D-dimensional hyperspherical surfaces of radii R_{n-1} and R_n. Site 1 is the boundary. (The general case of a hyperspherical boundary of arbitrary radius is considered in Ref. [4].) At time t walker at site n at time $t - 1$ moves outward to site $n + 1$ with probability $P_{\text{out}}(n)$ or inward to site $n - 1$ with probability $P_{\text{in}}(n)$. A walker at $n = 1$ must move outward: $P_{\text{out}}(1) = 1$, $P_{\text{in}}(1) = 0$. The D-dimensional random walk in Eq. (2) is now expressed by the one-dimensional recursion relation

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$$G_{n,t} = \begin{cases} zP_{\rm in}(n+1)G_{n+1,t-1} + zP_{\rm out}(n-1)G_{n-1,t-1} & (n \geq 3), \\ zP_{\rm in}(3)G_{3,t-1} + aG_{n-1,t-1} & (n = 2), \\ zP_{\rm in}(2)G_{2,t-1} & (n = 1). \end{cases} \quad (3)$$

The probabilities $P_{\rm out}(n)$ and $P_{\rm in}(n)$ must enforce local conservation of probability: $P_{\rm out}(n) + P_{\rm in}(n) = 1$. It is natural to take $P_{\rm out}(n)$ and $P_{\rm in}(n)$ to be in proportion to the hyperspherical surface areas crossed at each step [3]. Thus, if $S_D(R) = 2\pi^{D/2}R^{D-1}/\Gamma(D/2)$ represents the surface area of a D-dimensional hypersphere, then, for $n > 1$,

$$P_{\rm out}(n) = \frac{S_D(R_n)}{S_D(R_n) + S_D(R_{n-1})} \quad \text{and} \quad P_{\rm in}(n) = \frac{S_D(R_{n-1})}{S_D(R_n) + S_D(R_{n-1})}. \quad (4)$$

However, for dimensions other than $D = 1$ or 2, when we take $R_n = n$ the difference equation (3) cannot be solved in closed form [5]. Thus, we proposed [6] that the probabilities in Eqs. (4) be replaced by bilinear functions of n, which are uniformly good approximations to $P_{\rm out}(n)$ and $P_{\rm in}(n)$ in the range $D > 0$ when $R_n = n$:

$$P_{\rm out}(n) = \frac{n + D - 2}{2n + D - 3} \quad \text{and} \quad P_{\rm in}(n) = \frac{n - 1}{2n + D - 3}. \quad (5)$$

This crucial simplification in $P_{\rm in}$ and $P_{\rm out}$ preserves the configurational entropy [7] and gives

$$G_{n,t} = z^t \frac{\Gamma(\frac{D+1}{2})\Gamma(n + D - 2)}{2^{n-2}\Gamma(D)\Gamma(n + \frac{D-3}{2})} \oint_C \frac{dy}{2\pi i y}\, y^{n-t-1} \frac{(\frac{z}{a})^{\delta_{1,n}}\, {}_2F_1(\frac{n}{2}, \frac{n+1}{2}; n + \frac{D-1}{2}; y^2)}{1 + (\frac{z}{a} - 1)\, {}_2F_1(\frac{1}{2}, 1; \frac{D+1}{2}; y^2)}, \quad (6)$$

a closed-form solution of Eq. (3) for all $D > 0$. From Eq. (6) we can then obtain exact closed-form expressions for the spatial and temporal moments of the random walk [7].

To study critical behavior in the random-walk models in Eq. (2) or (3), we take the fraction of walkers at the boundary $\mathbf{0}$ (the site where random walkers are born) as the *order parameter.* Let $N_t = \sum_{\mathbf{n}} G_{\mathbf{n},t}$ be the total number of walkers at time t (N_0 is finite so N_t exists for all t). Then, $F_t = G_{\mathbf{0},t}/N_t$ is the fraction of all random walkers at site $\mathbf{0}$ at time t.

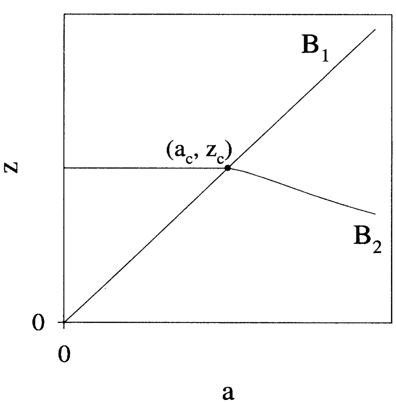

FIG. 1. Generic phase diagram for the (a, z) plane. Shown in the diagram are the boundary curves B_1 and B_2. To the left of B_1 and on B_1, the fraction F_t of random walkers at site $\mathbf{0}$ approaches 0 as $t \to \infty$; to the right of B_1 this fraction approaches a finite positive number as $t \to \infty$. Above B_2 the total number of random walkers, N_t, diverges as $t \to \infty$; below B_2 the total number of walkers approaches 0 as $t \to \infty$. On B_2 the distribution of random walkers approaches a steady state as $t \to \infty$. The critical point $(a_c, z_c = 1)$ lies at the intersection of B_1 and B_2.

The large-t asymptotic behaviors of N_t and F_t are determined by a and z regardless of the choice of $G_{\mathbf{n},0}$. We obtain a generic (lattice-independent) result: The positive quadrant of the (a, z) plane is partitioned into four distinct regions by boundary curves, B_1 and B_2, as shown in Fig. 1. The curve B_1 is a straight line passing through the origin. To the left of B_1, $F_t \to 0$ as $t \to \infty$; to the right of B_1, F_t approaches a positive finite value as $t \to \infty$. When $D \leq 2$ the equation for the line B_1 is $z = a$; as D increases beyond 2, this line remains straight, but its slope begins to decrease with increasing D. The transition at $D = 2$ is a reflection of Polya's theorem [8], which states that when $D > 2$ the probability of an individual random walker returning to an initial site is less than unity.

The left part of B_2 (the second boundary curve in Fig. 1) is a line segment, $z = 1$, connecting the z axis to the boundary line B_1. The right part of B_2 is a curve that approaches $z = 0$ as $a \to \infty$. The equation for the right part depends on D. [For a $D = 1$ lattice, where the probabilities of moving left or right are both $\frac{1}{2}$, this curve is given by $z = 2a/(a^2 + 1)$ $(a \geq 1)$.] Above B_2, $N_t \to \infty$ as $t \to \infty$; below B_2, $N_t \to 0$ as $t \to \infty$. On B_2 the total number of walkers approaches a finite value $N(a)$ as $t \to \infty$. On the curved portion of B_2, $N(a) > 0$ for $D > 2$, while $N(a) = 0$ for $D \leq 2$. This transition at $D = 2$ is yet another manifestation of Polya's theorem. The interpretation of a finite and nonzero $N(a)$ is that the distribution $G_{\mathbf{n},t}$ approaches a steady state, where there is a balance between random walkers being created at site $\mathbf{0}$ and annihilated at all other sites.

Across B_1, $\lim_{t\to\infty} F_t$ as $t \to \infty$ is continuous. We focus on the behavior of this limit as we cross B_1 along the boundary curve B_2 because it is only on B_2 that a steady state is reached as $t \to \infty$. Along B_2, $F(a) =$

$\lim_{t\to\infty} F_t$ undergoes a second-order phase transition at the critical point $(a_c, z_c = 1)$, which is situated at the intersection of B_1 and B_2. On B_2, $F(a) = 0$ where $a < a_c$ (even though the limiting value of N_t may be 0), and both $N(a)$ and $F(a)$ are finite positive numbers when $a > a_c$. The curved portion of B_2 is the locus of points in the (a, z) plane for which both $N(a)$ and $F(a)$ are finite and nonzero.

The universal features of Fig. 1 follow from Eq. (2). To determine B_1 we change variables: $G_{\mathbf{n},t} = z^t H_{\mathbf{n},t}$. The distribution $H_{\mathbf{n},t}$ represents a random walk with birth rate a/z at site $\mathbf{0}$ and no births or deaths at other sites (death rate 1). For such a walk, let $\mathbf{\Pi_0}$ be the probability that a walker at site $\mathbf{0}$ will ever return to $\mathbf{0}$. Then, of the $H_{\mathbf{0},0}$ walkers who begin at $\mathbf{0}$, only a fraction $\mathbf{\Pi_0}$ of them will return to $\mathbf{0}$ to give birth to new walkers. Of these new walkers, again only $\mathbf{\Pi_0}$ of them will return to $\mathbf{0}$, and so on. Hence, the total number of walkers ever born is the sum of a geometric series whose geometric ratio is $a\mathbf{\Pi_0}/z$. If $a\mathbf{\Pi_0}/z < 1$, the geometric series converges and the total number of walkers ever born is finite. As time t increases, the walkers diffuse away from site $\mathbf{0}$. Thus, as $t \to \infty$, the ratio $F_t = G_{\mathbf{0},t}/\sum_{\mathbf{n}} G_{\mathbf{n},t} = H_{\mathbf{0},t}/\sum_{\mathbf{n}} H_{\mathbf{n},t}$ vanishes. In contrast, if $a\mathbf{\Pi_0}/z > 1$, both $H_{\mathbf{0},t}$ and $\sum_{\mathbf{n}} H_{\mathbf{n},t}$ diverge at the same rate and $\lim_{t\to\infty} F_t$ lies between 0 and 1.

The transition between $F_t \to 0$ and $F_t \to$ *finite limit* occurs on the line $z = a\mathbf{\Pi_0}$, which is the boundary line B_1. Thus, since $z_c = 1$ for all $D > 0$, we find $a_c = 1/\mathbf{\Pi_0}$. Polya's theorem (which states that for any random walk $\mathbf{\Pi_0} = 1$ when $D \le 2$, and $\mathbf{\Pi_0} < 1$ when $D > 2$) explains the transition in the slope of the line B_1 at $D = 2$.

The shape of the curved part of B_2 depends on the choice of lattice and is not universal, but the straight part of B_2, $z = 1$ $(a < a_c)$, is universal and is easy to explain. Points (a, z) with $a < a_c$ and z near 1 lie to the left of B_1. Thus, F_t vanishes as $t \to \infty$. Hence, the effect of the birth rate a on the total number of walkers is negligible. The growth or decay of the total number of walkers depends only on z; if $z < 1$ then $\lim_{t\to\infty} N_t = 0$, and if $z > 1$ then $N_t \to \infty$ as $t \to \infty$. On the straight part of B_2 the limiting value of N_t depends on D. If $D \le 2$ then $a_c = 1$. Thus, on the left part of B_2 a fraction $1 - a$ of walkers who arrive at site $\mathbf{0}$ at a given time step must die at the next time step. But *all* walkers visit site $\mathbf{0}$ repeatedly (Polya's theorem), so N_t must vanish as $t \to \infty$. However, if $D > 2$ then $\mathbf{\Pi_0} < 1$. Thus, the fraction $1 - \mathbf{\Pi_0}$ of walkers who originate at site $\mathbf{0}$ *never return* to $\mathbf{0}$. These walkers never die because $z = 1$. Hence, N_t approaches a positive number as $t \to \infty$.

The form of the transition changes at $D = 4$. When $D < 4$ the slope of B_2 is continuous, but when $D > 4$ an elbow appears in B_2 at the critical value a_c. Specifically, when $D > 4$ the slope of B_2 is 0 for $0 \le a < a_c$; just above a_c the slope abruptly becomes $-\mathbf{\Pi_0}/(T - 1)$, where T is the expected time for a walker who begins at site $\mathbf{0}$ to return to $\mathbf{0}$ when $a = 1$ and $z = 1$. To prove this result [7] note that T, the first temporal moment of $C_{\mathbf{0},t;\mathbf{0}}$, is infinite when $D < 4$ and finite when $D > 4$. In a $z = 1$ model, only the fraction $\mathbf{\Pi_0}$ of walkers who leave site $\mathbf{0}$ ever return and walkers who return to $\mathbf{0}$ do so in T steps on average. Here, $z \ne 1$, so returning walkers experience a death rate z for $T - 1$ of these T steps. Thus, the expected number of walkers who actually return to $\mathbf{0}$ is reduced by the factor z^{T-1}. Hence, after T steps the number of walkers at $\mathbf{0}$ is multiplied by the factor $a\mathbf{\Pi_0}z^{T-1}$. The steady-state condition is thus $a\mathbf{\Pi_0}z^{T-1} = 1$. Near the critical point $a = a_c + \delta$ and $z = 1 - \epsilon$ as $\delta, \epsilon \to 0^+$. To first order in $\delta > 0$ and $\epsilon > 0$, the steady-state condition gives the slope of B_2 as $a \to a_c^+$. [The above argument is only valid near a_c, but the same reasoning yields the entire curve $z(a)$ in the limit $D \to \infty$. When $D = \infty$, $T = 2$ and $z(a) = a_c/a$].

To determine the nature of the phase transition in $F(a)$ along B_2, we let $g_{\mathbf{n}} = \lim_{t\to\infty} G_{\mathbf{n},t}$. The steady-state distribution $g_{\mathbf{n}}$ satisfies the difference equation

$$g_{\mathbf{n}} = \begin{cases} z \sum_{\{\sigma\}_{\mathbf{n}}} P(\sigma \to \mathbf{n}) g_\sigma & (\mathbf{n} \notin \{\sigma\}_{\mathbf{0}}), \\ aP(\mathbf{0} \to \mathbf{n}) g_{\mathbf{0}} + z \sum_{\{\sigma \ne \mathbf{0}\}_{\mathbf{n}}} P(\sigma \to \mathbf{n}) g_\sigma & (\mathbf{n} \in \{\sigma\}_{\mathbf{0}}), \end{cases} \tag{7}$$

which is the time-independent version of Eq. (2). For a steady-state solution having a finite number of walkers, the sum $\sum_{\mathbf{n}} g_{\mathbf{n}}$ exists and is nonzero. Summing Eq. (7) over all sites gives $\sum_{\mathbf{n}} g_{\mathbf{n}} = (a - z) g_{\mathbf{0}} + z \sum_{\mathbf{n}} g_{\mathbf{n}}$, from which we obtain $F(a)$ in terms of a and $z(a)$:

$$F(a) = \frac{g_{\mathbf{0}}}{\sum_{\mathbf{n}} g_{\mathbf{n}}} = \frac{1 - z(a)}{a - z(a)}. \tag{8}$$

Equation (8) is valid on the curved part of B_2 and on the straight part of B_2 when $D > 2$. Note that on B_2 we regard z as a function of a and treat F as a function of a only.

We have studied Eq. (7) for several types of lattices. We have found that along the curve B_2 the steady-state distribution fraction $F(a)$ behaves like $F(a) \sim C(D)(a - a_c)^\nu$ as $a \to a_c^+$ $(D \ne 2, 4)$. The multiplicative constant $C(D)$ depends on the specific choice of lattice. However, the critical exponent ν is universal and only depends on the dimension D. Using the probabilities in Eq. (5) for the hyperspherical lattice, we derive [7]

$$\nu = \begin{cases} D/(2 - D) & (0 < D < 2), \\ 2/(D - 2) & (2 < D < 4), \\ 1 & (D > 4). \end{cases} \tag{9}$$

We have verified that the second-order phase transition at a_c is universal by computing ν numerically for three types of random walks not analytically tractable: (i) a spherically symmetric random walk using the probabilities in Eqs. (4), (ii) a conventional random walk on a $D = 3$ cubic lattice, and (iii) a random walk on a fractal lattice

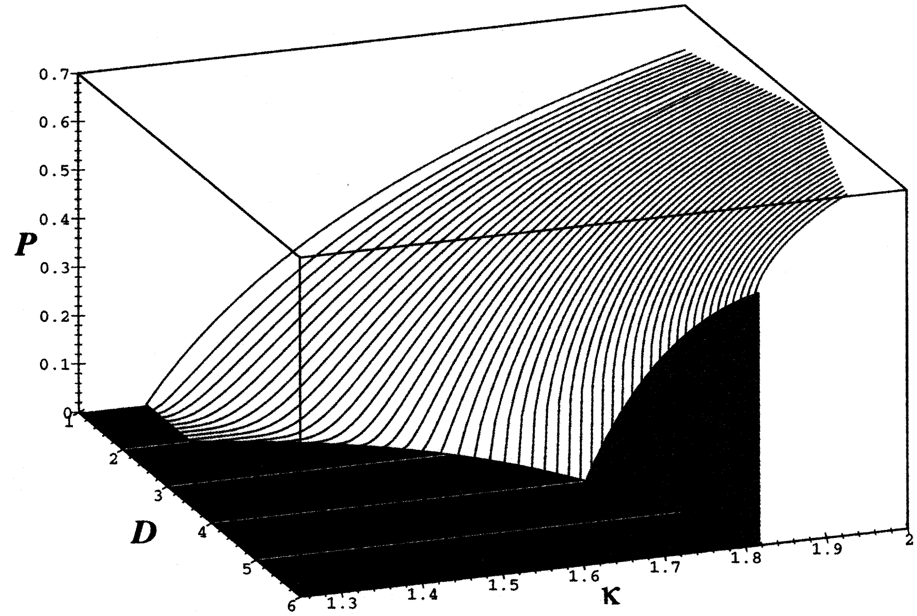

FIG. 2(color). Plot of the adsorption fraction $P(\kappa)$. For increasing $D < 2$, the scaling exponent increases and the transition becomes weaker until at $D = 2$ exponential scaling is obtained. For increasing $D > 2$, the scaling exponent decreases and the transition becomes stronger again; this is accompanied by an increase in the critical binding potential κ required to cause the transition. At $D = 4$ we observe a tricritical point with logarithmic scaling. For $D > 4$ to transition is first order, indicated by discontinuity (green shaded region) in $P(\kappa)$ across the critical point.

(Sierpinski carpet) and [9] with dimension $D = \ln 12/\ln 4$. Numerical agreement between the predicted value of ν in Eq. (9) and that obtained by computer simulation provides strong evidence of universality.

There is no critical exponent for the special cases $D = 2, 4$; for the case of a spherically symmetric random walk using the probabilities in Eq. (5), we find that [7] as $a \to a_c^+$

$$F(a) \sim \begin{cases} \frac{\text{const}}{a-a_c} e^{-2/(a-a_c)} & (D = 2), \\ \frac{a-a_c}{12\ln(\frac{1}{a-a_c})} & (D = 4). \end{cases} \qquad (10)$$

This work can be applied to the study of polymer growth in the vicinity of an attractive boundary [10]. For a hyperspherical boundary of radius m, this phenomenon is described by a partial difference equation of the same form as that in Eq. (7) [5]. If $P(\kappa)$ represents the fraction of a polymer that is adsorbed as a function of the attractive boundary potential κ, this fraction is analogous to $F(a)$ in Eq. (8). The potential κ is a monotonic function of the birth rate a, and near the critical point [4]

$$P(\kappa) \propto -\frac{dz(a)}{da} \sim C(D)\,(a - a_c)^{\nu'}. \qquad (11)$$

We find that $\nu' = \nu$ $(D < 2)$ and $\nu' = \nu - 1$ $(D > 2)$, where ν is given in Eq. (9). Thus, the polymer adsorption fraction $P(\kappa)$ exhibits a first-order transition for $D > 4$ and a tricritical point with logarithmic scaling at $D = 4$. This behavior for $P(\kappa)$ is illustrated in Fig. 2.

The analysis in this paper allows us to make a physical prediction for systems where excluded-volume effects can be neglected: The adsorption fraction for a solution of polymers growing near an approximately spherical attractive boundary (such as a cell membrane) exhibits a second-order phase transition with linear scaling.

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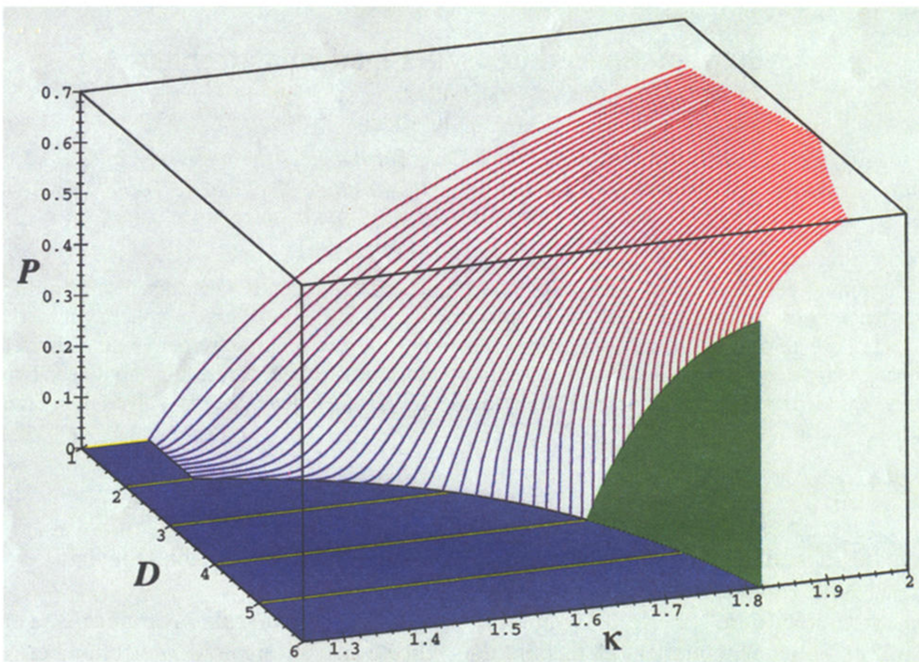

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