Generalized self-avoiding walk

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It is shown that the true self-avoiding walk problem in two dimensions admits introduction of two pseudoscalar charges in addition to the three scalar charges which were introduced by Obukhov and Peliti [J. Phys. A **16**, L147 (1983)]. These charges describe the nonequivalence of the left-hand and the right-hand turns during a two-dimensional walk. The renormalization-group equations are obtained for all five charges and the absence of stable fixed points for these equations is demonstrated. This absence of stable fixed points indicates that the symmetry breaking between the left-hand and the right-hand turns leads effectively to a walk with attraction and to localization.

It was shown recently by Amit, Parisi, and Peliti[1] that the self-avoiding walk problem is not simply a synonym for the problem of a random chain with excluded volume (see, for example, Ref. 2) but that it is rather an independent problem with higher critical dimension $d_c = 2$. The first two perturbative corrections, divergent at $d \leqslant 2$, were found in Ref. 1 and then used together with the assumptions of renormalizability and uniqueness of the charge g (interaction constant) to find for $d = 2$ the asymptotic dependence $\langle R^2 \rangle \sim N \ln^{2/5} N$, where $\langle R^2 \rangle$ is the mean square of the displacement and N is the number of steps. A diagrammatic technique which simplifies calculations of higher-order terms was developed by Obukhov and Peliti[3] for this problem and it was shown that the problem is characterized in general by three independent charges. The case considered in Ref. 1 should be described by the two-charge part of the general renormalization group and, hence, has a different assymptotic behavior, $\langle R^2 \rangle \sim N \ln N$.

The following formulation of the self-avoiding walk problem appears to be the simplest.[1] Let us assume that a traveler walks randomly over sites of a d-dimensional lattice trying to avoid those sites which he has already visited. Revisiting of sites cannot be completely forbidden because this would allow configurations of the paths in which the traveler would lock himself in. It is therefore assumed that the probability of a step from a site i to a neighboring site j depends on the number n_j of previous visits to th site j in the following way:

$$P_{i\to j} = \exp(-gn_j) \Big/ \sum_j \exp(-gn_j) \equiv \exp(g\nabla n_j(\mathbf{x}_i - \mathbf{x}_j)) \Big/ \sum_j \exp(\ldots), \quad \nabla n_j \equiv (n_i - n_j)(\mathbf{x}_i - \mathbf{x}_j)/(\mathbf{x}_i - \mathbf{x}_j)^2, \tag{1}$$

that is, for $g > 0$ this probability decays exponentially with increasing number of previous visits. Expression (1) is written taking into account the normalization condition for the probabilities $P_{i\to j}$, which assures that the traveler cannot come to rest at any given point.

Surface adsorption of a long polymer from a solution might be a physical example of a self-avoiding random walk. Suppose that one end of a long polymer is already attached to the surface. It is then clear that the segments closest to this end would be adsorbed next (Fig. 1). If this process is sufficiently slow relative to the relaxation of the spatial configuration, each newly adsorbed monomer will be attached randomly to the surface. Since it is assumed that different monomers repel each other this process can be considered a self-avoiding random walk on a plane, described by the transition probability (1).

We shall briefly describe the origin of the diagrammatic rules which were formulated without any derivation in Ref. 3. This will help us to understand the meaning of the charges $g_1, \ldots, g_5$ which we shall discuss below. We first suppose that the number of self-intersections is small when the number of steps is not too large and we consider only the effect of a single intersection on the unperturbed correlation function. Let $G_N(\mathbf{x},\mathbf{x}')$ be the probability of arriving at $\mathbf{x}'$ after n steps originating at $\mathbf{x}$. In the zeroth approximation

$$G_N^{(0)}(\mathbf{x}-\mathbf{x}') = \frac{1}{(4\pi N)^{d/2}} \exp\left[-\frac{(\mathbf{x}-\mathbf{x}')^2}{2Nd}\right]. \tag{2}$$

We will consider the simplest configuration with a single intersection[1)] (Fig. 2).

The probability that during a walk a traveler passing through a point $\mathbf{x}_1$ will pass at a later time through a point $\mathbf{x}_2$ near it is

$$P(\mathbf{x}, \mathbf{x}_1, \mathbf{x}_2) = G_N(\mathbf{x}-\mathbf{x}_1) G_N(\mathbf{x}_1-\mathbf{x}_2), \quad |\mathbf{x}_1-\mathbf{x}_2| = a. \tag{3}$$

Here N_1 and N_2 are the numbers of steps completed between the points $\mathbf{x}$ and $\mathbf{x}_1$ and between $\mathbf{x}_1$ and $\mathbf{x}_2$, respectively, while a is the lattice constant; the expression (3) will later be

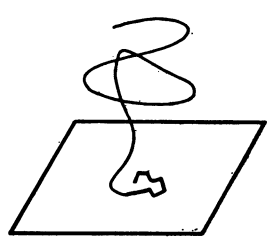

FIG. 1.

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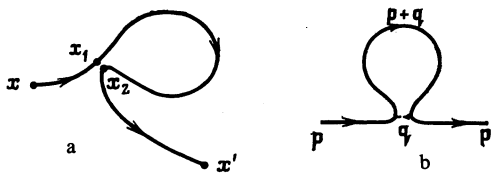

FIG. 2.

summed over all possible N_1 and N_2. The walk is not free at the point $\mathbf{x}_2$ but proceeds according to the probability (1). The mean displacement at that step is

$$\mathbf{a}=g(\mathbf{x}_1-\mathbf{x}_2)/|\mathbf{x}_1-\mathbf{x}_2|,$$

and, taking into account the probability (3) of the entire configuration, we have

$$\langle\mathbf{a}\rangle=\mathbf{a}P(\mathbf{x},\ \mathbf{x}_1,\ \mathbf{x}_2). \tag{4}$$

Let us expand $P(\mathbf{x},\mathbf{x}_1,\mathbf{x}_2)$ in the small difference $\mathbf{x}_1-\mathbf{x}_2$ and sum over all possible directions of the difference $\mathbf{x}_1-\mathbf{x}_2$. In the continuous limit we obtain

$$\langle\mathbf{a}\rangle=g\nabla_{\mathbf{x}_1}G_{N_1}(\mathbf{x}-\mathbf{x}_1)G_{N_2}(\mathbf{x}_1-\mathbf{x}_2)\,|_{\mathbf{x}_1\to\mathbf{x}_2}. \tag{5}$$

Therefore, a path with a single self-intersection differs from a purely free one in that a displacement by $\langle\mathbf{a}\rangle$ occurs at the point $\mathbf{x}_2$. This displacement changes the probability of landing after N_3 steps at a final point $\mathbf{x}'$ by

$$\delta G=\langle\mathbf{a}\rangle\nabla_{\mathbf{x}_2}G_{N_3}(\mathbf{x}_2-\mathbf{x}'). \tag{6}$$

By summing the correction (6) over all possible positions of the point $\mathbf{x}_2$ in which a self-intersection occurred, and over all possible N_1, N_2 and N_3 such that $\Sigma N_i=N$, $i=1,2,3$, we obtain the the first-order correction to the random-walk expression (2). If we go over to the momentum representation and take the Laplace transform with respect to the variable N,

$$G(\tau,\mathbf{p})=\sum_N G_N(\mathbf{p})e^{-\tau N}, \tag{7}$$

it turns out that the correction to $G^{(0)}(\tau,\mathbf{p})$ is described by the diagram of Fig. 2b, where the lines are associated with the correlation functions $G^{(0)}(\tau,\mathbf{p})$ and the vertices are associated with the expression $g(\mathbf{q}\cdot\mathbf{p})$.

All further corrections can be expressed as a diagrammatic series with vertices $g(\mathbf{q},\mathbf{p}'-\mathbf{q})$ (Fig. 3). In such vertices it is necessary to distinguish between the lines of the preceding (I) and succeeding (II) passages through the intersection point.

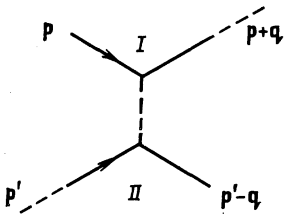

FIG. 3.

An expression with a different combination of momenta, $g_2(\mathbf{p}',\mathbf{p}'-\mathbf{q})$, occurs in the first-order perturbation theory for the effective vertex. Therefore, in order to sum higher-order terms in the perturbation theory it is necessary to write renormalization-group equations for two charges g_1 and g_2. In addition, a charge g_3 with the momentum structure $(\mathbf{p},\mathbf{p}'-\mathbf{q})$ is also possible. Such a charge occurs if it is assumed that upon approaching an interesection point the traveler prefers to proceed along (or contrary to) his previous path at that point. In the case of polymer adsorption this means that the parallel (or antiparallel) packing of polymer segments occurring at a single point is preferred. Such a situation is described by the transition probability

$$P_{i\to j}=\exp\{g(\mathbf{m}(\mathbf{x}_j),\ \mathbf{x}_i-\mathbf{x}_j)\}\Big/\sum_j\exp\{g(\mathbf{m}(\mathbf{x}_j),\ \mathbf{x}_i-\mathbf{x}_j)\}, \tag{8}$$

where $\mathbf{m}(\mathbf{x}_j)$ is the flux of previous visits to the point $\mathbf{x}_j$. Should we begin with (8), we obtain by a derivation analogous to (3)–(6) a diagrammatic technique with the vertices $g_1(\mathbf{q},\mathbf{p}'-\mathbf{q})$ and $g_3(\mathbf{p},\mathbf{p}'-\mathbf{q})$.

The renormalization-group equations for all three charges g_1, g_2, and g_3 and arbitrary d were written out in Ref. 3. In recent lectures Peliti[4] introduced a field theory within which these equations can be formally derived. Because the interaction vertices of this theory are proportional to the second power of the momenta, the upper critical dimension for the problem is $d=2$ instead of $d=4$ in the usual φ^4 theory. Therefore, excluding cases of exotic walks on fractal lattices, the only nontrivial and physically realizable cases are $d=1$ and $d=2$. The case $d=1$ is not trivial as might appear at first sight. It was considered in Ref. 5 by one of us. The dimension $d=2$ appears most interesting for the self-avoiding walk problem.

Furthermore, the expressions quadratic in the moments can be written in any other dimension by using only the operation of the scalar product. In that case the set of charges g_1, g_2, and g_3 is complete since the interaction vertex is uniquely described by three momenta, $\mathbf{q}$, $\mathbf{p}$, and $\mathbf{p}'$, which can be multiplied scarlarly only with the next outgoing momentum $\mathbf{p}'-\mathbf{q}$ (II) in Fig. 3). The reason for the latter is causality: a self-intersection affects only the subsequent travel.

In the two-dimensional case a pseudoscalar quadratic in the momenta can be written using the vector product. One of the momenta in this product must be $\mathbf{p}'-\mathbf{q}$. Consequently there are only two independent combinations, such as $g_4[\mathbf{q}(\mathbf{p}'-\mathbf{q})]$ and $g_5[\mathbf{p}(\mathbf{p}'-\mathbf{q})]$, where the charges g_4 and g_5 are pseudoscalars while $[\mathbf{ab}]\equiv\mathbf{a}\tilde{\mathbf{b}}$ and $\tilde{b}_\mu\equiv\varepsilon_{\mu\nu}b_\nu$ is the vector dual to $\mathbf{b}$, $\varepsilon_{\mu\nu}$ being the unit antisymmetric tensor. These pseudoscalar charges appear in the discrete formulation of the problem if it is assumed that the transition probabilities are

$$P_{i\to j}=\exp[g(\nabla n_j,\tilde{\mathbf{a}}_{ij})]\Big/\sum_j\exp[g(\nabla n_j,\tilde{\mathbf{a}}_{ij})] \tag{9}$$

or

$$P_{i\to j}=\exp[g(\mathbf{m}_j\tilde{\mathbf{a}}_{ij})]\Big/\sum_j\exp[g(\mathbf{m}_j\tilde{\mathbf{a}}_{ij})],\quad \mathbf{a}_{ij}\equiv\mathbf{x}_i-\mathbf{x}_j \tag{10}$$

respectively. In order to clarify the origin and properties of

the probabilities (9) it is useful to note that they can be obtained from a more general transition probability which depends on the density of previous visits not only to the points i and j, but also to the neighboring points:

$$P_{i\to j}=\Big(\sum_j \exp[\ldots]\Big)^{-1}\exp[f_1 n_i+f_2 n(\mathbf{x}_i+\tilde{\mathbf{a}}_{ij})+f_3 n(\mathbf{x}_i-\tilde{\mathbf{a}}_{ij})$$

$$+f_4 n(\mathbf{x}_i+\mathbf{a}_{ij})-f_5 n_j-f_6 n(\mathbf{x}_j+\tilde{\mathbf{a}}_{ij})+f_7 n(\mathbf{x}_j-\tilde{\mathbf{a}}_{ij})+f_8 n(\mathbf{x}_j-\mathbf{a}_{ij})]$$

$$\approx\Big(\sum_j \exp[\ldots]\Big)^{-1}\exp[g(\nabla n_j,\mathbf{a}_{ij})+\tilde{g}(\nabla n_j,\tilde{\mathbf{a}}_{ij})],\quad(11)$$

where

$$g=\sum_{k=4}^{8} f_k+f_8,\quad \tilde{g}=f_2-f_3-f_6+f_7.$$

In writing the second equality in (11) we restricted ourselves to the leading terms of the expansion in powers of ∇n_i of the argument of the exponential. If the walk problem corresponding to (11) is invariant with respect to the reflection $\tilde{\mathbf{a}}_{ij}\to -\tilde{\mathbf{a}}_{ij}$ or to the product of this reflection and the transformation $i\leftrightarrow j, f_i\to -f_i$, then $\tilde{g}=0$ and (11) reduces to (1). If, however, the problem is not invariant relative to these transformations, then $\tilde{g}\neq 0$ and (11) reduces to the product of (1) and (9). We see in this way that the transition probability of the type (9) occurs in problems of walks with broken left-right symmetry. A realization of such a situation could be, for example, a walk of a charged particle in a magnetic field.

The self-avoiding walk problem can also be understood as a problem of scattering of the walking particle by inhomogeneities created by its preceding walk. It is also possible to assume that these inhomogeneities already existed on the lattice. In the case of polymer surface adsorption, these are simply the inhomogeneities of the adsorbing surface. The inhomogeneities can also be created by the polymers previously adsorbed on the surface. In the latter case the problem is described by the transition probabilities of the type (1), where n_j is some random function defined on the lattice. We will denote this quantity by $\bar{n}_j$ in order to distinguish it from the number of previous visits to the site j. The quantity $g\nabla\bar{n}$ is the mean displacement at a given point. If on the average $\langle\nabla\bar{n}\rangle\neq 0$, which in case of the polymer adsorption could mean a tilt of the adsorbing surface or a steady solvent flow along the surface, the problem reduces for long distances to the problem of a drifting free walk. If

$$\langle\nabla\bar{n}\rangle=0,\quad \langle\nabla\bar{n}(\mathbf{x}),\nabla\bar{n}(\mathbf{x}')\rangle=2g\delta(\mathbf{x}-\mathbf{x}'),$$

it is not difficult to see that an effective interaction describable with the vertex $g(\mathbf{p}+\mathbf{q},\mathbf{p}'-\mathbf{q})$ arises (see Fig. 3). A free walk over an inhomogenous surface reduces in this fashion to the problem of a self-avoiding walk with $g_1=g_3=g$.

Analogous generalizations are possible for walks on a lattice with transition probabilities of the type (8), where $\bar{\mathbf{m}}$ is now a random vector field specified on the lattice. It is known that an arbitrary vector field can be represented as

$$\bar{\mathbf{m}}=\nabla u+\tilde{\nabla}v,\quad \tilde{\nabla}_\mu=\varepsilon_{\mu\nu}\nabla_\nu,\quad \mu,\nu=1,2,$$

where u and v are the scalar and "vector" potentials, respectively. If only the pair correlations of the irrotational (longitudinal)

$$\langle\nabla_\mu u(\mathbf{x}),\quad \nabla_\nu u(\mathbf{x}')\rangle$$

and the solenoidal (transverse)

$$\langle\tilde{\nabla}_\mu v(\mathbf{x}),\quad \tilde{\nabla}_\nu v(\mathbf{x}')\rangle$$

parts of the field are nonzero, then the problem reduces to the one considered above. In particular, when the mean curl of the field $\bar{\mathbf{m}}$ is nonzero this leads only to a renormalization of the diffusion constant. If, however, the crossed correlations

$$\langle\nabla_\mu u(\mathbf{x})\quad \tilde{\nabla}_\nu v(\mathbf{x}')\rangle,$$

are nonzero the problem of a walk with $g_4,g_5\neq 0$ occurs.

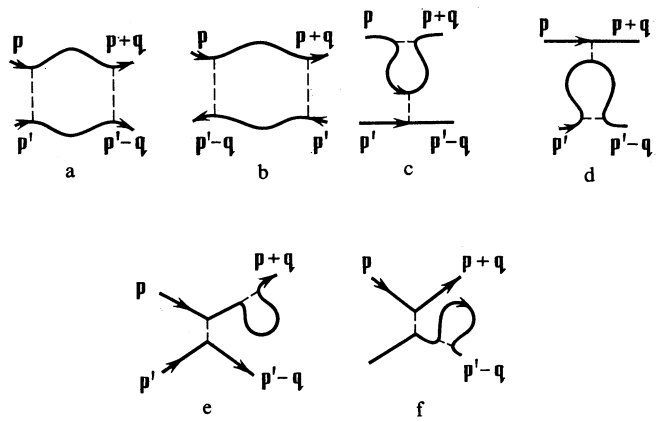

FIG. 4.

In order to derive the renormalization-group equations for the general walk problem we introduce the complete vertex

$$\Gamma(\mathbf{p},\mathbf{p}',\mathbf{q})=g_1(\mathbf{q},\mathbf{p}'-\mathbf{q})+g_2(\mathbf{p}',\mathbf{p}'-\mathbf{q})+g_3(\mathbf{p},\mathbf{p}'-\mathbf{q})$$
$$+g_4[\mathbf{q}(\mathbf{p}'-\mathbf{q})]+g_5[\mathbf{p}(\mathbf{p}'-\mathbf{q})]$$

and calculate its one-loop logarithmic corrections (Fig. 4). As a result we obtain the following system of equations:

$$\begin{aligned}
dg_1/d\xi&=-{}^5/_2 g_1^2+2g_1g_2+3g_1g_3-{}^1/_2 g_2^2-{}^1/_2 g_4^2,\\
dg_2/d\xi&=(g_1-g_3)(g_1-3g_2)+g_2^2+g_4(g_5-g_4),\\
dg_3/d\xi&={}^5/_2 g_3^2-2g_1g_3+g_2g_3+{}^1/_2 g_5^2-g_4g_5,\\
dg_4/d\xi&=g_4(2g_2+g_3)+g_2g_5,\qquad dg_5/d\xi=g_5(-g_1+2g_2+2g_3),
\end{aligned}\quad(12)$$

where $\zeta=\ln t=-\ln\max(N^{-1},|\mathbf{p}|,|\mathbf{p}'|,|\mathbf{q}|)$.

The complete system of equations (12) allows for several self-consistent decreases of the number of variables. That is, if the initial values of some charges are zero they will remain so. We call such simplifications reductions of the system of equations. We observe first that for $g_4=g_5=0$ the equations (12) reduce to the general equations for the three scalar charges g_1, g_2, and g_3 obtained in Ref. 3. They have two reductions: $g_3=0$ and $g_1=g_2=0$. Besides these reductions, the system (12) allows for the reductions with nonzero pseudoscalar charges g_4 and g_5:

I. $g_1=g_2=g_4=0$, $g_3, g_5\neq 0$;

II. $g_3=g_5=0$, $g_1, g_2, g_4\neq 0$;

III. $g_5=0$, $g_1, g_2, g_3, g_4\neq 0$.

If the pseudoscalar charges are set equal to zero, we return to the corresponding reductions of the scalar system.

We will now analyze the system (12). It can be shown that the complete system (12) has no nontrivial fixed points. This means that the asymptotic behavior of a random walk, which is determined by the renormalized diffusion coefficient $D_R(t)$,

$$\langle R^2\rangle \sim D_R(t)\,t, \quad D_R(t)=D_0\exp\int\frac{(g_1-g_3)\,dt}{t}$$

cannot have a purely power-law character except in the case of a free walk where $\langle R^2\rangle \sim D_0 t$. To determine the logarithmic corrections to the asymptotic behavior it is convenient to exploit the homogeneity of the system (12) by transforming to equations for "charges" $\gamma_i = g_i/\xi$. They are

$$\begin{aligned} d\gamma_1/d\eta&=\gamma_1-{}^5/_2\gamma_1^2+2\gamma_1\gamma_2+3\gamma_1\gamma_3-{}^1/_2\gamma_2^2-{}^1/_2\gamma_4^2,\\ d\gamma_2/d\eta&=\gamma_2+(\gamma_1-\gamma_3)(\gamma_1-3\gamma_2)+\gamma_2^2+\gamma_4(\gamma_5-\gamma_4),\\ d\gamma_3/d\eta&=\gamma_3+{}^5/_2\gamma_3^2-2\gamma_1\gamma_3+\gamma_2\gamma_3+{}^1/_2\gamma_5^2-\gamma_4\gamma_5,\\ d\gamma_4/d\eta&=\gamma_4+\gamma_4(2\gamma_2+\gamma_3)+\gamma_2\gamma_5, \quad d\gamma_5/d\eta=\gamma_5(1-\gamma_1+2\gamma_2+2\gamma_3), \end{aligned} \tag{13}$$

where $\eta = \ln\xi$. To each fixed point of the system (13) corresponds a solution of (12) which has the form $g_i(\xi)\sim\gamma_i^*/\xi$, $\xi\gg 1$. It is obvious that the system (13) admits of the same reductions as the system (12).

Equations (13) have only scalar nontrivial fixed points: 1) $\gamma_1^*=\gamma_2^*=1$; 2) $\gamma_3^*=-2/5$; 3) $\gamma_1^*=-\gamma_2^*=1/5$; 4) $\gamma_1^*=\gamma_2^*/2=2$; 5) $\gamma_1^*=\gamma_2^*/3=\gamma_3^*/4=1/11$. In these points all other γ_i^* are equal to zero. In the absence of pseudoscalar charges the fixed points 1) and 2) are stable and give the asymptotic behavior $\langle R^2\rangle \sim t\ln t$ and $\langle R^2\rangle \sim t\ln^{2/5}t$, respectively. If, on the other hand, the initial values $g_{40}, g_{50}\neq 0$, then all the fixed points are unstable. Hence, all the charges go off to infinity with time, corresponding to the strong-coupling regime. This behavior of the solutions of the equations (12) and (13) is confirmed by our computer simulations of these equations.

In the realm of applicability of our equations it is of interest to consider the influence of small pseudoscalar charges ($g_{40}, g_{50} \ll g_{10,20,30}$) on the behavior of the scalar charges which determine the asymptotic behavior of $\langle R^2\rangle$ near the stable fixed points 1) and 2). It is sufficient to consider not the complete system of equations (12) but only its reductions I and II. We will consider them separately.

I. In this case when $g_5 = 0$ there is a stable fixed point $\gamma_2^* = -2/5$ which corresponds to a logarithmic decrease $g_3(\xi)\sim 2/5\xi$, $\xi\gg 1$. Introduction of the pseudoscalar charge g_5 changes the picture. A simple analysis of the system of equations for two charges g_3 and g_5 shows that for initial values satisfying the conditions $g_{50}\ll|g_{30}|\ll 1$ the charge g_3 at first decreases logarithmically until $\xi^*\sim(g_{50})^{-5}$ and then follows a different behavior. It follows from the exact solution of this system that the real quantity is

$$\xi_1^*\sim[g_{50}(g_{50}/g_{30})^4]^{-1}\equiv A^{-1}\ll\xi^*$$

(in view of the initial conditions), while the charges g_3 and g_5 begin to grow to infinity after passing respectively through zero and through a minimum equal to A (note that our equations are not applicable for values of g_i of the order of 1). This behavior of the charges means that up to times of order $t^*\sim\exp(b/A)$, where b is a nonuniversal constant of order unity, the asymptotic behavior of $\langle R^2\rangle$ is determined by the fixed point γ_3^*. This is followed by a change of the asymptotic regime in which the further behavior is determined by the strong-coupling region. Exponentially large t^* mean that the change of the asymptotic regime occurs at very large times difficult to be reached in ususal numerical simulations of random walks. We remark that the correlation length has an analogous (exponential) behavior (with a square root singularity however) in the high-temperature vicinity of phase transition points of the Berezinskiĭ-Kosterlitz-Thouless type.[6]

II. In this case, when $g_4 = 0$ there is a stable fixed point $\gamma_1^*=\gamma_2^*=1$ which also corresponds to a logarithmic decrease $g_{1,2}(\xi)\sim 1/\xi$, $\xi\gg 1$.

An analysis analogous to the one given in (I) shows that for $g_{40}\ll g_{10}\approx g_{20}\ll 1$ there are also two asymptotic regimes, the first one being logarithmic and extending to $t^*\sim\exp(b/A)$, where $A\sim(g_{40})^{1/3}$.

For completeness we remark that analogous, two-regime behavior of the scalar charges occurs also in the absence of both pseudoscalar charges when the initial charges g_{i0}, $i = 1,2,3$, are near the singly-unstable fixed point. In this case a walk with the asymptotic behavior $\langle R^2\rangle\sim N\ln^{3/11}t$ proceeds up to a time of the order $t^*\sim\exp(b\Delta^{-\nu})$ where Δ is the initial deviation of g_{i0} from the critical surface containing the fixed point 5 and $\nu = 1/\lambda_+$, $\lambda_+ = 1/11$ being the unstable exponent of the fixed point 5.

Therefore, we see that introduction of pseudoscalar charges can change the asymptotic behavior of a true random walk. While in the case of purely scalar charges there is in the phase space of the charges a region of initial values g_{i0} such that in a sufficiently large time a particle can move arbitrarily far away from the origin, introduction of pseudoscalar charges leads to a localization which corresponds to the behavior of the scalar charges found in points I and II.

In conclusion, we emphasize that our derivation is correct only in the region of validity of the equations (12).

[1)]By self-intersection we will mean here the case when a point of the walk occurs near its previous path so that the walk is not free at that point, but takes place with the probability distribution (1).

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