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A note on configurational properties of constrained random walks

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Abstract. This paper is a collection of examples showing various effects on configurational properties of a random walk under the constraint that the ends of the random walk be fixed. Some formalism is developed for the solution of such problems, allowing us to express results in terms of the characteristic function of the unconstrained random walk. Several applications of this formalism are made in the paper. Typical of these is the result that fixing the ends of a random walk with an underlying stable-law density forces the steps of the resulting walk to have a number of finite moments. Other results show a range of differences to be expected between properties of constrained and unconstrained random walks.

1. Introduction

The problem of determining configurational properties of polymer chains under constraints, exemplified by the requirement that the two ends of the chain be held a fixed distance apart, has been tackled by a number of investigators beginning with the work of Kuhn and his collaborators [1-4]. A variety of related problems phrased in terms of diffusion was analysed by Hollingsworth [5]. Recently, Weiss and Rubin [6] have discussed configurational properties of span-constrained random walks, while Domb [7] has used generating functions to calculate spatial moments for constrained random walks. The work of Kuhn *et al* and that of Domb produce no qualitative differences between the results for constrained and those for unconstrained random walks because of the nature of the questions asked. Hollingsworth [5], on the other hand, investigated the effects of fixing the endpoints of a random flight on the probability of its passing close to one or more specified points during its course. In his investigation the form of this probability does differ from the simple Gaussian that is characteristic of the unconstrained flight. Hollingsworth, however, did not discuss any detailed consequences of his results. Other problems related to conditioning of random walks have been analysed, among others, by Bolthausen [8], Pakes [9], Rubin and Weiss [10], and Doney [11].

In this paper, we consider some examples of effects of a specific class of constraints on configurational properties of continuum random walks. Our results relate mainly to effects produced by requiring that the end-to-end distance of an n-step random flight be a fixed vector. A further example demonstrates some effects of fixing both the first and second moments of a specific random walk.

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In the absence of constraints the steps of the random walk will be assumed to be independent and identically distributed. The presence of a constraint, of course, introduces correlations between the individual steps so that tools developed for random walks with independent steps cannot be used without some modification. We examine the nature of these correlations as well as their effects on the probability density of the intermediate steps. It will be seen, for example, that when the steps of an unconstrained random walk have a stable-law distribution with no finite moments, then the requirement that the random walk passes through a fixed point at step n implies the existence of higher-order moments for the probability density of single steps $m \leq n$. In another calculation we show that the imposition of constraints on the first two moments of a random walk with zero-mean Gaussian steps implies that the probability density for a single step of the constrained random walk has a form drastically different from the original Gaussian. Thus, the effects of even rather simple constraints can lead to significant qualitative changes in the resulting behaviour of the constrained random walk.

In a companion paper [12], we discuss the effect of fixing the end-to-end vector on the number of distinct sites visited by an n-step lattice random walk, where the constraint will also be seen to cause effects that differ substantially from those calculated for unconstrained walks.

Several closely related kinds of constraints have been treated in the random walk literature. An example is provided by the calculation of properties of random walks constrained to remain within a specified region [13]. The present work suggests a somewhat different range of problems posed by the imposition of constraints, and proves a rich lode of interesting problems for further consideration.

2. Characteristic functions and moments

The focus of this paper is on the determination of properties of single-step and joint transition densities for a constrained random walk. These will be discussed in terms of the characteristic function for the underlying unconstrained random walk. Let $p(\boldsymbol{r})$ be the probability density function for the displacement in a single step of an unconstrained random walk in D dimensions with independent and identically distributed steps. We will initially suppose that a single constraint of the form

$$\boldsymbol{r}_1 + \boldsymbol{r}_2 + \ldots + \boldsymbol{r}_n = \boldsymbol{v} \tag{2.1}$$

is imposed on the random walk. The set of random variables of interest will be the partial sums $\boldsymbol{S}_m = \boldsymbol{r}_1 + \boldsymbol{r}_2 + \ldots + \boldsymbol{r}_m$, $m \leq n$. However, the principal configurational effects induced by the constraints are found in $\boldsymbol{S}_1 (= \boldsymbol{r}_1)$, so that we focus mainly on this quantity.

We therefore denote by $q_n(\boldsymbol{r}|\boldsymbol{v})$ the probability density of a single displacement under the constraint imposed by (2.1), and denote by $p_n(\boldsymbol{v})$ the probability density for the unconstrained random walk to reach v at step n. The conditional density can then be expressed as

$$q_n(\boldsymbol{r}|\boldsymbol{v}) = \frac{p(\boldsymbol{r})}{p_n(\boldsymbol{v})} \int \ldots \int p(\boldsymbol{r}_2) p(\boldsymbol{r}_3) \ldots p(\boldsymbol{r}_n) \delta\Big(\sum_i \boldsymbol{r}_i - \boldsymbol{v}\Big) \, \mathrm{d}^D \boldsymbol{r}_2 \ldots \mathrm{d}^D \boldsymbol{r}_n \tag{2.2}$$

where, in the delta function representing the effect of the constraint, we set $\boldsymbol{r}_1 \equiv \boldsymbol{r}$ and where the integration is over all space for each of the variables. Although we have set $\boldsymbol{r}_1 = \boldsymbol{r}$, the $\boldsymbol{r}_j$ appear symmetrically in the sum so that $q_n(\boldsymbol{r}|\boldsymbol{v})$ represents the step density for any of the $\boldsymbol{r}_j$. If we insert the Fourier representation of the delta function

$$\delta(\boldsymbol{r}) = \frac{1}{(2\pi)^D} \int_{-\infty}^{\infty} \exp(-\mathrm{i}\boldsymbol{\omega}\cdot\boldsymbol{r})\,\mathrm{d}^D\boldsymbol{\omega} \tag{2.3}$$

into the expression for $q_n(\boldsymbol{r}|\boldsymbol{v})$, and use the characteristic function defined by

$$C(\boldsymbol{\omega}) = \int_{-\infty}^{\infty} p(\boldsymbol{r}) \exp(\mathrm{i}\boldsymbol{\omega}\cdot\boldsymbol{r})\,\mathrm{d}^D\boldsymbol{r} \tag{2.4}$$

then we find that $q_n(\boldsymbol{r}|\boldsymbol{v})$ is

$$\begin{aligned} q_n(\boldsymbol{r}|\boldsymbol{v}) &= \frac{p(\boldsymbol{r})}{(2\pi)^D p_n(\boldsymbol{v})} \int_{-\infty}^{\infty} \exp[\mathrm{i}\boldsymbol{\omega}\cdot(\boldsymbol{r}-\boldsymbol{v})] C^{n-1}(\boldsymbol{\omega})\,\mathrm{d}^D\boldsymbol{\omega} \\ &= p(\boldsymbol{r}) p_{n-1}(\boldsymbol{v}-\boldsymbol{r})/p_n(\boldsymbol{v}) \end{aligned} \tag{2.5}$$

where

$$p_n(\boldsymbol{v}) = \frac{1}{(2\pi)^D} \int_{-\infty}^{\infty} \exp(-\mathrm{i}\boldsymbol{\omega}\cdot\boldsymbol{v}) C^n(\boldsymbol{\omega})\,\mathrm{d}^D\boldsymbol{\omega}. \tag{2.6}$$

The characteristic function that can be associated with $q_n(\boldsymbol{r}|\boldsymbol{v})$ is

$$\begin{aligned} C_n(\boldsymbol{\rho}|\boldsymbol{v}) &= \langle \exp(\mathrm{i}\boldsymbol{\rho}\cdot\boldsymbol{S}_1) | \boldsymbol{S}_n = \boldsymbol{v} \rangle \\ &= \int_{-\infty}^{\infty} q_n(\boldsymbol{r}|\boldsymbol{v}) \exp(\mathrm{i}\boldsymbol{\rho}\cdot\boldsymbol{r})\,\mathrm{d}^D\boldsymbol{r} \\ &= \frac{1}{(2\pi)^D} \frac{1}{p_n(\boldsymbol{v})} \int_{-\infty}^{\infty} C(\boldsymbol{\omega}+\boldsymbol{\rho}) C^{n-1}(\boldsymbol{\omega}) \exp(-\mathrm{i}\boldsymbol{\omega}\cdot\boldsymbol{v})\,\mathrm{d}^D\boldsymbol{\omega}. \end{aligned} \tag{2.7}$$

In a similar fashion we can associate the characteristic function

$$\begin{aligned} C_{m,n}(\boldsymbol{\rho}|\boldsymbol{v}) &= \langle \exp(\mathrm{i}\boldsymbol{\rho}\cdot\boldsymbol{S}_m) | \boldsymbol{S}_n = \boldsymbol{v} \rangle \\ &= \frac{1}{(2\pi)^D} \frac{1}{p_n(\boldsymbol{v})} \int_{-\infty}^{\infty} \exp(-\mathrm{i}\boldsymbol{\omega}\cdot\boldsymbol{v}) C^m(\boldsymbol{\omega}+\boldsymbol{\rho}) C^{n-m}(\boldsymbol{\omega})\,\mathrm{d}^D\boldsymbol{\omega} \end{aligned} \tag{2.8}$$

with the partial sum $\boldsymbol{S}_m$.

This representation of the characteristic function has at least one obvious and simple consequence, namely that the first moment of the displacement is always finite for step numbers $\leqslant n$, regardless of whether the unconstrained random walk has an average single-step displacement that is finite or not. This can be seen from the formula for the average sum of the first m steps,

$$\langle \boldsymbol{S}_m | \boldsymbol{S}_n = \boldsymbol{v} \rangle = m\boldsymbol{v}/n \tag{2.9}$$

which is obtained from (2.4) and (2.8) as

$$\langle (\boldsymbol{S}_m)_l | \boldsymbol{S}_n = \boldsymbol{v} \rangle = -\mathrm{i} \left. \frac{\partial C_{m,n}(\boldsymbol{\rho}|\boldsymbol{v})}{\partial \rho_l} \right|_{\boldsymbol{\rho}=\boldsymbol{0}} \tag{2.10}$$

where $(\boldsymbol{S}_m)_l$ is the lth component of $\boldsymbol{S}_m$. These first moments are determined solely by the constraint and by no other property of the unconstrained random walk. This is not, of course, true for higher moments, which will indeed depend on the specific $p(\boldsymbol{r})$.

It is instructive to consider the limit distribution derivable from (2.8) for $n \to \infty$. For simplicity, we restrict ourselves to a one-dimensional random walk in which the steps of the unconstrained random walk have a finite mean, μ, and a finite variance, σ^2. The limiting densities of S_m, $m \leq n$, will be found in the limits $n, m \gg 1$, in which one can use an argument familiar in random walk theory based on the approximation

$$C(\omega) \sim \exp(\mathrm{i}\mu\omega - \tfrac{1}{2}\sigma^2\omega^2) \qquad \omega \to 0. \tag{2.11}$$

This expansion allows us to infer the validity of the central limit theorem in the present context. Indeed, on making the approximation of (2.11) in both the numerator and denominator of (2.8) we find that

$$C_{m,n}(\rho \mid v) \sim \exp[imv\rho/n - \tfrac{1}{2}m(1-m/n)\sigma^2\rho^2] \qquad m, n \to \infty \tag{2.12}$$

which is the characteristic function corresponding to a Gaussian distribution for S_m, the mean and variance of which are

$$\langle S_m \mid S_n = v \rangle = mv/n \qquad \sigma^2(S_m \mid S_n = v) \sim m(1-m/n)\sigma^2. \tag{2.13}$$

It is interesting to observe that the bias parameter, μ, does not appear in the expression given in (2.12). This has a deeper reason which is explained in [12]. Note that the expression for $\sigma^2(S_m \mid S_n = v)$ has the correct qualitative behaviour in that it is equal to 0 when $m = 0, n$ and reaches a maximum when $m = n/2$. It is evident from this last equation that $\sigma^2(S_m \mid S_n = v)$ is asymptotically independent of v which implies that the qualitative features of the constrained random walk are unchanged when v is allowed to depend on n.

3. Stable-law densities

3.1. *The Cauchy walk*

An interesting effect arises in the case of stable-law walks. Let us examine the particular case of a one-dimensional random walk in which the component steps have a Cauchy density

$$p(x) = 1/[\pi(1+x^2)] \tag{3.1}$$

which has a characteristic function $C(\omega) = \exp(-|\omega|)$ and for which the density for the sum of n steps is

$$p_n(x) = n/[\pi(n^2+x^2)]. \tag{3.2}$$

In this simple example, we can find the probability density for a single step, x, of the constrained random walk by evaluating the integral in (2.5) exactly. One finds that

$$q_n(x \mid v) = \frac{(n-1)(n^2+v^2)}{\pi n(1+x^2)} \frac{1}{[(n-1)^2+(v-x)^2]}. \tag{3.3}$$

As we have mentioned, $q_n(x \mid v)$ must have at least one finite moment. It is evident from this expression that $q_n(x \mid v)$ has both a finite first and second moment, but not a finite third moment since $q_n(x \mid v)$ goes like x^{-4} for large x^2. The mean and variance of a single step are found to be

$$\langle S_1 \mid S_n = v \rangle = v/n \qquad \sigma^2(S_1 \mid S_n = v) = (n-1)(1+v^2/n^2). \tag{3.4}$$

It is readily verified from the first representation of $q_n(r \mid v)$ given in (2.5) that the probability density for the sum of $m \leq n$ constrained Cauchy random variables also vanishes for large x^2 as x^{-4} so that the variance is finite also in this case, but not the third moment. It is of interest to compute the constrained variance, $\sigma^2(S_m\,|\,S_n=v)$ for the constrained Cauchy random walk. The exact result is

$$\sigma^2(S_m\,|\,S_n=v)=m(n-m)(1+v^2/n^2) \tag{3.5}$$

which may be compared to the large m, n result given in (2.12) for the finite-variance random walk. As is the case there, the maximum variance occurs when $m\sim n/2$. If v is also allowed to depend on v, say $v=v_0n^\beta$, a qualitative change occurs in the dependence on n. When m is held fixed and n increased, the order of the variance is n, provided that $\beta\leqslant 1$. However, when $\beta>1$ the order of the n dependence is greater than n. This change of behaviour also occurs in the correlation function calculated later in (3.19).

3.2. General stable-law walks

Our remarks leading to (3.4) suggest the problem of finding the number of finite moments of a constrained random walk when the unconstrained walk has a stable-law form, i.e. $p(x)\sim|x|^{-(\alpha+1)}$, $0<\alpha\leqslant 2$, $|x|\to\infty$. For such densities, the characteristic function has the property that $C(\omega)\sim\exp(-|\omega|^\alpha)$, $\omega\to 0$, from which we can infer, from (2.5), that

$$q_n(x\,|\,v)\sim|x|^{-2(\alpha+1)} \qquad x\to\infty. \tag{3.6}$$

Thus the numbers of finite moments for the constrained random walk whose steps are characterised by such stable-law densities are 1 for $0<\alpha\leqslant\frac{1}{2}$, 2 for $\frac{1}{2}<\alpha\leqslant 1$, 3 for $1<\alpha\leqslant\frac{3}{2}$ and 4 for $\frac{3}{2}<\alpha\leqslant 2$. These results are valid not only for the single-step densities, but also for the density of the sum S_m for all $m\leqslant n$.

Similar results can be found for stable-law random walks in higher dimensions. Rather than trying to examine a very general case, we willl analyse a particular example in two dimensions, namely,

$$p(\boldsymbol{r})=\frac{\beta a^{2\beta}}{2\pi}\frac{1}{(r^2+a^2)^{1+\beta}} \tag{3.7}$$

where $r^2=x^2+y^2$. When $0<\beta\leqslant\frac{1}{2}$, $p(\boldsymbol{r})$ has no finite moments and when $\frac{1}{2}<\beta\leqslant 1$, it has exactly one. The characteristic function corresponding to $p(\boldsymbol{r})$ is

$$C(\boldsymbol{\omega})=C(\omega)=2\beta a^{2\beta}\int_0^\infty\frac{rJ_0(\omega r)}{(r^2+a^2)^{1+\beta}}\,\mathrm{d}r \tag{3.8}$$

in which $\omega^2=\omega_1^2+\omega_2^2$ and $J_0(x)$ is a zeroth-order Bessel function. The expression for $q_n\,(r\,|\,v)$ is given in (2.5), which in the present case will be written

$$q_n(\boldsymbol{r}\,|\,\boldsymbol{v})=\frac{p(\boldsymbol{r})}{2\pi p_n(\boldsymbol{v})}\,Q(R) \tag{3.9}$$

in which $R=|\boldsymbol{r}-\boldsymbol{v}|$ and $Q(R)$ is defined by

$$Q(R)=\int_0^\infty\omega C^{n-1}(\omega)J_0(\omega R)\,\mathrm{d}\omega. \tag{3.10}$$

The problem of determining the number of finite moments of $q_n(\boldsymbol{r}\,|\,\boldsymbol{v})$ therefore depends on the evaluation of $Q(R)$ in the limit of large R. An analysis given in the appendix shows that $Q(R)\sim R^{-2(1+\beta)}$ for $R\to\infty$, so that

$$q_n(\boldsymbol{r}\,|\,\boldsymbol{v})\sim r^{-4(1+\beta)}. \tag{3.11}$$

Hence, the number of finite moments for each step of the constrained random walk is 2 for $0<\beta\leqslant\frac{1}{4}$, 3 for $\frac{1}{4}<\beta\leqslant\frac{1}{2}$, 4 for $\frac{1}{2}<\beta\leqslant\frac{3}{4}$ and 5 for $\frac{3}{4}<\beta<1$.

4. Correlation functions

The existence of a constraint implies that the individual steps of the random walk must be correlated until the step at which the constraint is fulfilled. To examine and quantify this correlation, we develop the appropriate characteristic function formalism. Let $q_n(\boldsymbol{r}_1, \boldsymbol{r}_2|\boldsymbol{v})$ denote the joint density of two steps of the random walk. We note that because the $\boldsymbol{r}_j$ in (2.1) are interchangeable, we may choose any two steps to calculate the joint density; in other words, the joint density is the same for any pair of steps. On following the steps leading to (2.5) we find

$$q_n(\boldsymbol{r}_1, \boldsymbol{r}_2|\boldsymbol{v})=\frac{p(\boldsymbol{r}_1)p(\boldsymbol{r}_2)}{(2\pi)^D p_n(\boldsymbol{v})}\int_{-\infty}^{\infty}\exp\left[\mathrm{i}\boldsymbol{\omega}\cdot(\boldsymbol{r}_1+\boldsymbol{r}_2-\boldsymbol{v})\right]C^{n-2}(\boldsymbol{\omega})\,\mathrm{d}^D\boldsymbol{\omega}. \tag{4.1}$$

The corresponding characteristic function is

$$C_n(\boldsymbol{\rho}_1, \boldsymbol{\rho}_2|\boldsymbol{v})=\frac{1}{(2\pi)^D p_n(\boldsymbol{v})}\int_{-\infty}^{\infty}C(\boldsymbol{\omega}+\boldsymbol{\rho}_1)C(\boldsymbol{\omega}+\boldsymbol{\rho}_2)C^{n-2}(\boldsymbol{\omega})\exp(\mathrm{i}\boldsymbol{\omega}\cdot\boldsymbol{v})\,\mathrm{d}^D\boldsymbol{\omega}. \tag{4.2}$$

Without losing any qualitative features of the analysis we can again restrict ourselves to one dimension. A formal expression for the lowest-order mixed moment, $\langle x_1x_2|S_n=v\rangle$, can be obtained from (4.2) in integral form as

$$\langle x_1x_2|S_n=v\rangle=-\frac{1}{2\pi p_n(v)}\int_{-\infty}^{\infty}\exp(-\mathrm{i}\omega v)[C'(\omega)]^2C^{n-2}(\omega)\,\mathrm{d}\omega. \tag{4.3}$$

Let us examine the behaviour of the covariance function $\langle x_1x_2|S_n=v\rangle-\langle x_1|S_n=v\rangle\times\langle x_2|S_n=v\rangle$ as a function of n, on the assumption that the first two moments of $p(x)$ are finite. In the limit $n\to\infty$, we may replace $C(\omega)$ by its form for $p(x)$, a Gaussian with mean equal to μ and variance σ^2. It is possible then to evaluate $C_n(\rho_1, \rho_2|v)$, and we get

$$C_n(\rho_1, \rho_2|v)\sim\exp\left(\mathrm{i}(\rho_1+\rho_2)\frac{v}{n}-\frac{\sigma^2}{2}(\rho_1^2+\rho_2^2)+\frac{\sigma^2}{2n}(\rho_1+\rho_2)^2\right) \tag{4.4}$$

which is independent of μ as one might expect it to be [12]. The correlations come from the last term in the exponent which is proportional to n^{-1}. The specific form of the correlation function derived from (4.4) is

$$\langle x_1x_2|S_n=v\rangle-\langle x_1|S_n=v\rangle\langle x_2|S_n=v\rangle\sim-\sigma^2/n. \tag{4.5}$$

The associated variance is

$$\sigma^2(x|S_n=v)\sim\sigma^2(n-1)/n \tag{4.6}$$

which is slightly less than the unconstrained value, which in the present case is exactly equal to σ^2. It is reasonable to conjecture in general that the variance calculated with a linear constraint will always be less than the unconstrained variance for v fixed and $n\to\infty$, but we have been unable to settle this question in any generality.

It is interesting to repeat this calculation for a distribution which has no moments. For simplicity, we consider only the Cauchy density given in (3.1). In this case, since $C(\omega)$ has such a simple form, it follows that

$$C_n(\rho_1, \rho_2 | S_n = v) = \frac{n^2+v^2}{2n} \int_{-\infty}^{\infty} \exp[-|\omega+\rho_1| - |\omega+\rho_2| - (n-2)|\omega| - \mathrm{i}\omega v]\, \mathrm{d}\omega \tag{4.7}$$

so that

$$\langle x_1 x_2 | S_n = v\rangle - \langle x_1 | S_n = v\rangle\langle x_2 | S_n = v\rangle = 1 - v^2/n^2 \tag{4.8}$$

which demonstrates the intuitively evident fact that constrained stable-law walks tend to be more highly correlated than random walks whose underlying densities have finite moments. Equation (4.8) is remarkable from two points of view. The first is that it approaches a positive limit as $n \to \infty$, in contrast to the result given in (4.5). This contradicts the intuitively plausible notion that the covariance should decrease as n increases, since one expects the constraint to become less stringent for large n. This is indeed the case when the mean and variance of the unconstrained walk are finite as illustrated in (4.6). In the present case, however, because a large step induces further larger steps in order to satisfy the constraint, the covariance tends to a finite limit at large step numbers.

5. Some generalisations

There are a number of generalisations of the preceding analysis that are amenable to development along the lines described earlier. One of these replaces the simple constraint of (2.1) by a scalar constraint of the form

$$\sum_{i=1}^{n} f(\boldsymbol{r}_i) = F \tag{5.1}$$

where $f(\boldsymbol{r}_j)$ is a scalar function and F is a constant. This condition can be incorporated by means of a delta function into the integral representation of $q_n(\boldsymbol{r}|f,F)$. In this case, one finds

$$q_n(\boldsymbol{r}|f, F) = p(\boldsymbol{r}) \int_{-\infty}^{\infty} \exp[\mathrm{i}\omega(f(\boldsymbol{r}) - F)] B^{n-1}(\omega)\, \mathrm{d}\omega \left(\int_{-\infty}^{\infty} \exp(-\mathrm{i}\omega F) B^n(\omega)\, \mathrm{d}\omega \right)^{-1} \tag{5.2}$$

where

$$B(\omega) = \int_{-\infty}^{\infty} p(\boldsymbol{r}) \exp(\mathrm{i}\omega f(\boldsymbol{r}))\, \mathrm{d}^D \boldsymbol{r}. \tag{5.3}$$

Vector constraints can be introduced in exactly the same manner through the use of a product of delta functions.

Qualitatively interesting effects occur also in the case of multiple constraints, as will be seen by the following simple example. We assume that the underlying single-step density is a one-dimensional zero-mean Gaussian, which we take to be $p(x) = (2\pi)^{-1/2} \exp(-x^2/2)$. Let us constrain both the n-step mean and variance of the random walk by requiring that

$$\sum_{i=1}^{n} x_i = X \qquad \sum_{i=1}^{n} x_i^2 = S^2. \tag{5.4}$$

We will calculate the probability density for a single step of the constrained random walk. This function will be denoted by $q_n(x|X, S^2)$ and is given by the ratio of two functions which have nearly the same form:

$$q_n(x|X, S^2) = N_n(x, X, S^2)/p_n(X, S^2) \tag{5.5}$$

where

$$\begin{aligned} N_n(x, X, S^2) &= \frac{\exp(-x^2/2)}{(2\pi)^{n/2}} \int_{-\infty}^{\infty} \exp\left(-\tfrac{1}{2}\sum_2^n x_i^2\right) \delta\left(\sum_1^n x_i - X\right) \delta\left(\sum_1^n x_i^2 - S^2\right) \mathrm{d}x_2 \ldots \mathrm{d}x_n \\ p_n(X, S^2) &= \frac{1}{(2\pi)^{n/2}} \int_{-\infty}^{\infty} \exp\left(-\tfrac{1}{2}\sum_1^n x_i^2\right) \delta\left(\sum_1^n x_i - X\right) \delta\left(\sum_1^n x_i^2 - S^2\right) \mathrm{d}x_2 \ldots \mathrm{d}x_n. \end{aligned} \tag{5.6}$$

The method for evaluating these integrals is an extension of that used in § 2. We evaluate the integral for $p_n(X, S^2)$ as an illustration.

By introducing Fourier integral representations of the two delta functions into (5.6) we find

$$p_n(X, S^2) = \frac{1}{4\pi^2} \int_{-\infty}^{\infty} \int \exp(-\mathrm{i}\omega_1 X - \mathrm{i}\omega_2 S^2) J^n(\omega_1, \omega_2)\, \mathrm{d}\omega_1\, \mathrm{d}\omega_2 \tag{5.7}$$

where

$$\begin{aligned} J(\omega_1, \omega_2) &= \frac{1}{(2\pi)^{1/2}} \int_{-\infty}^{\infty} \exp(-\tfrac{1}{2}x^2 + \mathrm{i}\omega_1 x + \mathrm{i}\omega_2 x^2)\, \mathrm{d}x \\ &= \frac{1}{(1-2\mathrm{i}\omega_2)^{1/2}} \exp\left(-\frac{\omega_1^2}{2(1-2\mathrm{i}\omega_2)}\right). \end{aligned} \tag{5.8}$$

Substitution of (5.8) into (5.7) allows us to perform the integration over ω_1. In this way, we find that $p_n(X, S^2)$ can be represented as a single integral of the form

$$p_n(X, S^2) = \frac{1}{(2\pi)^{3/2}} \frac{\exp(-x^2/2n)}{n^{1/2}} \int_{-\infty}^{\infty} \frac{\exp[-\mathrm{i}\omega(S^2 - X^2/n)]}{(1-2\mathrm{i}\omega)^{(n-1)/2}}\, \mathrm{d}\omega. \tag{5.9}$$

A simple way to evaluate this integral is to introduce the representation

$$\frac{1}{(1-2\mathrm{i}\omega)^{(n-1)/2}} = \frac{1}{\Gamma((n-1)/2)} \int_{-\infty}^{\infty} t^{(n-3)/2} \exp[-t(1-2\mathrm{i}\omega)]\, \mathrm{d}t \tag{5.10}$$

followed by an easily justified interchange of orders of integration. We then find

$$\begin{aligned} p_n(X, S^2) &= \frac{1}{(2\pi)^{3/2} n^{1/2}} \frac{\exp(-X^2/2n)}{\Gamma((n-1)/2)} \int_0^{\infty} t^{(n-3)/2} \exp(-t)\, \mathrm{d}t \\ &\quad \times \int_{-\infty}^{\infty} \exp[-\mathrm{i}\omega(s^2 - X^2/n - 2t)]\, \mathrm{d}\omega \\ &= \frac{1}{(2\pi n)^{1/2}} \frac{\exp(-X^2/2n)}{\Gamma((n-1)/2)} \int_0^{\infty} t^{(n-3)/2} \exp(-t) \delta(S^2 - X^2/n - 2t)\, \mathrm{d}t \\ &= \frac{1}{(2\pi n)^{1/2}} \frac{1}{2^{(n-1)/2}\Gamma((n-1)/2)} (S^2 - X^2/n)^{(n-3)/2} \exp(-S^2/2). \end{aligned} \tag{5.11}$$

An expression for $N_n(x, X, S^2)$ can be found by using essentially the same technique. The resulting expression for the density $q_n(x, X, S^2)$ is

$$q_n(x|X, S^2) = \left(\frac{2n}{n-1}\right)^{1/2} \frac{\Gamma((n-1)/2)}{\Gamma((n-2)/2)} \frac{\{[S^2 - x^2 - (x-X)^2/(n-1)]_+\}^{n/2-1}}{(S^2 - X^2/n)^{(n-3)/2}} \tag{5.12}$$

where the symbol V_+ is defined by

$$V_+ = \begin{cases} V & V = 0 \\ 0 & V \leqslant 0. \end{cases}$$

The form for $q_n(x|X, S^2)$ shown in (5.12) differs qualitatively from a Gaussian because it has compact support and contains a polynomial rather than an exponential. This of course must be the case because of the constraint that the sum of squares is fixed. The ends of the interval over which $q_n(x|X, S^2)$ is non-zero are located at

$$x_\pm = (1/n)\{X \pm [m(n-1)(S^2 - X^2/n)]^{1/2}\} \tag{5.13}$$

and the maximum of $q_n(x|X, S^2)$ occurs at $x = X/n$. In the limit of large n the interval in x over which $q_n(x|X, S^2)$ is non-zero tends to $(-S, S)$.

One further relatively straightforward generalisation of the foregoing analysis replaces the sum in (2.1) by a linear combination of the r_j. That is to say,

$$\sum_{j=1}^{n} \alpha_j \boldsymbol{r}_j = \boldsymbol{v}. \tag{5.14}$$

In this case, (2.5) is changed to

$$q_n(\boldsymbol{r}_k|\boldsymbol{v}) = p(\boldsymbol{r}_k) \int_{-\infty}^{\infty} \exp[\mathrm{i}(\alpha_k \boldsymbol{r}_k - \boldsymbol{v}) \cdot \boldsymbol{\omega}] \prod_{\substack{j=1 \\ \neq k}}^{n} C(\alpha_j \boldsymbol{\omega}) \mathrm{d}^D \boldsymbol{\omega}$$
$$\times \left(\int_{-\infty}^{\infty} \exp(-\mathrm{i}\boldsymbol{v} \cdot \boldsymbol{\omega}) \prod_{j=1}^{n} C(\alpha_j \boldsymbol{\omega})\, \mathrm{d}^D \boldsymbol{\omega} \right)^{-1}. \tag{5.15}$$

Notice that here the particular $\boldsymbol{r}_j$ must be specified because the α_j in (5.14) removes the inherent symmetry between variables.

Just a few examples have been given to illustrate some of the rich variety of changes in configurational statistics of random walks consequent on the introduction of a constraint. Many other constraints naturally suggest themselves for further study. Of these, one case which appears to be of a higher order of difficulty, although not impossible, is the constraint that a lattice random walker reach a specified set for the first time at step n. A second related problem is to determine the effects of requiring the random walker to be in one of a set of sites at step n, or to be at a particular site at some time during the step number interval $(0, n)$.

Appendix

We give a heuristic derivation of the asymptotic behaviour of $Q(R)$ for large R. The expression for $Q(R)$ given in (3.10) indicates that the major contribution to the integral comes from the neighbourhood $\omega \sim 0$. This being true, we can return to (3.8) to find an approximation for $C(\omega)$ accurate for small ω. For this purpose, we can approximate the Bessel function in the integral representation of $C(\omega)$ by

$$J_0(\omega r) \sim 1 - (\omega r)^2/4 \sim \exp[-(\omega r)^2/4] \qquad \omega \to 0 \tag{A1}$$

so that

$$C(\omega)\sim 2\beta a^{2\beta}\int_0^\infty \frac{r\exp[-(\omega r)^2/4]}{(r^2+a^2)^{1+\beta}}\,\mathrm{d}r$$
$$=\beta\int_0^\infty \frac{\exp(-a^2\omega^2 v/4)}{(v+1)^{1+\beta}}\,\mathrm{d}v. \qquad \text{(A2)}$$

An integration by parts allows us to write

$$C(\omega)\sim 1-\left(\frac{a\omega}{2}\right)^2\int_0^\infty \frac{\exp(-a^2\omega^2 v/4)}{(v+1)^{\beta}}\,\mathrm{d}v. \qquad \text{(A3)}$$

The remaining integral on the right-hand side is in the form of a Laplace transform. To find its behaviour for ω^2 small, we use an Abelian theorem for Laplace transforms relating the small ω^2 behaviour to the large v behaviour of the integrand [14], exclusive of the exponential, i.e. $v^{-\beta}$. By following this prescription, we find

$$C(\omega)\sim 1-\Gamma(1-\beta)\left(\frac{a\omega}{2}\right)^{2\beta}$$
$$\sim \exp\left[-\Gamma(1-\beta)\left(\frac{a\omega}{2}\right)^{2\beta}\right]. \qquad \text{(A4)}$$

This implies that

$$Q(R)\sim\int_0^\infty \omega J_0(\omega R)\exp\left[-\Gamma(1-\beta)(n-1)\left(\frac{a\omega}{2}\right)^{2\beta}\right]\mathrm{d}\omega. \qquad \text{(A5)}$$

This representation for $Q(R)$ can be regarded as having come from an $(n-1)$-step random walk for which the characteristic function is that given in the last line of (A4). Thus, we may replace the exponential in (A5) by the exact expression for $C(\omega)$ in (3.8), with a suitably redefined constant which we denote by b. That is to say we let $b^{2\beta}=(n-1)\ a^{2\beta}$. By interchanging the order of integration, we then find

$$Q(R)\sim 2\beta b^{2\beta}\int_0^\infty \frac{r\,\mathrm{d}r}{(r^2+b^2)^{1+\beta}}\int_0^\infty \omega J_0(\omega r)J_0(\omega R)\,\mathrm{d}\omega \qquad R\to\infty. \qquad \text{(A6)}$$

However, the ω integral can be expressed in terms of a delta function:

$$\int_0^\infty \omega J_0(\omega r)J_0(\omega R)\,\mathrm{d}\omega=\frac{1}{r}\delta(r-R) \qquad \text{(A7)}$$

with the result that

$$Q(R)\sim 2\beta b^{2\beta}/(R^2+b^2)^{1+\beta}. \qquad \text{(A8)}$$

This shows that when n is held fixed and R tends towards ∞, $Q(R)\sim R^{-2(1+\beta)}$ as asserted.

References

[1] Kuhn W 1934 *Kolloid Zeit.* **68** 2
[2] Kuhn W and Kuhn H 1945 *Helv. Chim. Acta* **29** 1095
[3] Katchalsky A, Kuenzle O and Kuhn W 1950 *J. Polym. Sci.* **5** 283

[4] Volkenstein M V 1966 *Configurational Statistics of Polymer Chains* (New York: Wiley-Interscience)
[5] Hollingsworth C A 1952 *J. Chem. Phys.* **20** 1580
[6] Weiss G H and Rubin R J 1980 *J. Stat Phys.* **22** 97
[7] Domb C 1981 *J. Phys. A: Math. Gen.* **14** 219
[8] Bolthausen E 1976 *Ann. Prob.* **4** 480
[9] Pakes A G 1978 *J. Appl. Prob.* **15** 292
[10] Rubin R J and Weiss G H 1978 *Macromol.* **11** 1046
[11] Doney R A 1983 *J. Appl. Prob.* **20** 409
[12] den Hollander W Th F and Weiss G H 1988 *J. Appl. Prob.* to be published
[13] Weiss G H and Rubin R J 1983 *Adv. Chem. Phys.* **52** 363
[14] Doetsch G 1944 *Theorie und Anwendungen der Laplace Transformation* (New York: Dover)