DISCUSSION

WAYNE W. BARRETT

Texas A and M University

I would like to direct my comments to a few specific items in Professor Freed's paper. I found the exact formula for $\langle |\mathbf{R}|^2 \rangle$, the first equation in the paper, to be quite striking even though peripheral to the main part of the paper. It turns out that it can easily be derived using conditional expectations. Since

(1)
$$\langle |\mathbf{R}|^2 \rangle = \langle |\sum_{j=1}^n \mathbf{b}_j|^2 \rangle = \sum_{i=1}^n \sum_{j=1}^n \langle \mathbf{b}_i \cdot \mathbf{b}_j \rangle$$

it suffices to compute $\langle \mathbf{b}_i \cdot \mathbf{b}_j \rangle$. Now $\langle \mathbf{b}_i \cdot \mathbf{b}_{i+1} \rangle = b^2 \cos \omega$ where $\omega = \pi - \theta$ since $\mathbf{b}_i \cdot \mathbf{b}_{i+1} \equiv b^2 \cos \omega$. Assume inductively that $\langle \mathbf{b}_i \cdot \mathbf{b}_{i+k-1} \rangle = b^2 \cos^{k-1} \omega$. It is clear geometrically that

$$E(\mathbf{b}_{i+1} | \mathbf{b}_i) = \mathbf{b}_i \cos \omega$$

for all i.

Let
$$\mathscr{F}_i = \mathscr{F}(\mathbf{b}_1, \mathbf{b}_2, \dots, \mathbf{b}_i)$$
. Then

$$\langle \mathbf{b}_{i} \cdot \mathbf{b}_{i+k} \rangle = \langle E(\mathbf{b}_{i} \cdot \mathbf{b}_{i+k} | \mathscr{F}_{i+k-1}) \rangle$$

$$= \langle \mathbf{b}_{i} \cdot E(\mathbf{b}_{i+k} | \mathscr{F}_{i+k-1}) \rangle = \langle \mathbf{b}_{i} \cdot E(\mathbf{b}_{i+k} | \mathbf{b}_{i+k-1}) \rangle$$

$$= \langle \mathbf{b}_{i} \cdot \mathbf{b}_{i+k-1} \cos \omega \rangle = (b^{2} \cos^{k-1} \omega) \cos \omega$$

$$= b^{2} \cos^{k} \omega$$

by the properties of conditional expectation, the Markov property and the inductive hypothesis.

Therefore, $\langle \mathbf{b}_i \cdot \mathbf{b}_{i+k} \rangle = b^2 \cos^k \omega$ for all integers i and k by induction. Substituting in (1), the result follows by a straightforward calculation.

The quantity Z_N defined by equation (2.9) is proportional to the total number of walks given the excluded volume constraint. This can be understood as follows. For simplicity, let $J(r) = ((4/3) \pi \epsilon^3)^{-1} I_{B\epsilon}$ where $I_{B\epsilon}$ is the indicator function of the ball with center at the origin and radius ϵ . The essential thing is that J be an approximate δ function. Then

$$\begin{split} Z_n &= \Bigg[\prod_{i=1}^N \int_{\{|r_i-r_j|>\epsilon \text{ all } i\neq j\}} d\mathbf{r}_i\Bigg] G_0(\{\mathbf{r}_i\} \mid \mathbf{r}_0 \equiv 0) \mathrm{exp} \Bigg[-\frac{v}{2} \sum_{i\neq j=0}^N J(\mathbf{r}_i - \mathbf{r}_j)\Bigg] \\ &+ \Bigg[\prod_{i=1}^N \int_{\{|r_i-r_j|\leq\epsilon \text{ some } i\neq j\}} d\mathbf{r}_i\Bigg] G_0(\{r_i\} \mid \mathbf{r}_0 \equiv 0) \mathrm{exp} \Bigg[-\frac{v}{2} \sum_{i\neq j=0}^N J(\mathbf{r}_i - \mathbf{r}_j)\Bigg] \end{split}$$

The first term is $P\{|\mathbf{r}_i - \mathbf{r}_j| > \epsilon, \text{ all } i \neq j\}$, the probability in terms of $G_0(\{r_i\})$. The second term is positive and less than $\exp[-v((4/3)\pi\epsilon^3)^{-1}]$. Thus, for the second term to be negligible we need $v = c((4/3)\pi\epsilon^3)$ for large enough c. This indicates why v is called the excluded volume. Thus

$$Z_N \approx P\{|r_i - r_j| > \epsilon, \text{ all } i \neq j\}.$$

Now, if we let n_{EV} be the total number of walks under the Gaussian distribution satisfying the excluded volume restriction, and let n be the number of unrestricted walks (number of trials), then

$$\frac{n_{EV}}{n} \approx P\{|\mathbf{r}_i - \mathbf{r}_j| > \epsilon, \text{ all } i \neq j\}$$

and Z_N is, except for a small error, proportional to n_{EV} .