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Entanglement probabilities of polymers: a white noise functional approach

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Abstract

The entanglement probabilities for a highly flexible polymer to wind n times around a straight polymer are evaluated using white noise analysis. To introduce the white noise functional approach, the one-dimensional random walk problem is taken as an example. The polymer entanglement scenario, viewed as a random walk on a plane, is then treated and the entanglement probabilities are obtained for a magnetic flux confined along the straight polymer, and a case where an entangled polymer is subjected to the potential $V = \dot{f}(s)\vartheta$. In the absence of the magnetic flux and the potential V, the entanglement probabilities reduce to a result obtained by Wiegel.

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1. Introduction

Recently, white noise analysis was applied to evaluate the Feynman path integral for quantum systems with flat wall boundaries and topological constraints [1]. These include the infinite wall problem, the particle in a box, and topologically constrained systems exemplified by the quantum particle in a circle and the Aharonov–Bohm set-up. In this paper, we extend this white noise functional integral approach to statistical mechanics by treating entangled polymer systems. In 1967, Edwards [2] and, independently, Prager and Frisch [3], solved the entanglement problem of two chainlike macromolecules in the absence of intermolecular forces. The problem consists of a polymer on a plane whose motion is constrained by a straight polymer orthogonal to the plane, since the macromolecules cannot cross each other. The polymer on the plane has fixed endpoints and can be viewed as a random walk with paths that can entangle n times around the straight polymer which intersects the origin of the plane. Interesting quantities based on this entangled polymer were also investigated by Saito and Chen [4]. On the other hand, Wiegel [5] extended this entanglement problem to include an intermolecular force where the repeating units of the entangled polymer interact with the straight polymer. The force is repulsive at short distances and attractive at large distances

with the potential, $V = Cr^2 + D/r^2$ ($C > 0$, $D > 0$). Wiegel then obtained the entanglement probabilities for this harmonically bound polymer to be

$$W(n) = (R/l)\sqrt{4\pi/N}\exp(-4\pi^2 n^2 R^2/Nl^2) \qquad (N \gg 1) \tag{1.1}$$

where $R = (D/C)^{1/4}$, is the radius where the potential has a minimum, and the polymer is represented by N freely hinged rods, each of length l. For low temperatures, Wiegel also noted that the configurations of the polymer are confined to a narrow strip in the immediate vicinity of a circle around the origin with radius R. The result, equation (1.1), is also a low-temperature limit of entanglement probabilities for any potential $V(r)$ which has a minimum at some radius R.

We apply white noise analysis [6–9] in this paper by evaluating the entanglement probabilities for two other scenarios. The first, discussed in section 3, considers the case where the straight polymer perpendicular to the plane possesses a magnetic flux confined along its length. This appears to be a classical analogue of the Aharonov–Bohm effect [10] since the entanglement probability is affected by the confined magnetic flux, even if the entangled polymer lies in a region with zero magnetic field. We discuss the second case in section 4 where the entangled polymer on the plane is subjected to the potential, $V = \dot{f}(s)\vartheta$. Here, $\dot{f}(s) = \mathrm{d}f/\mathrm{d}s$, where $0 \leqslant s \leqslant L$ and L is the length of the polymer. As a specific example, we take $V = k\vartheta$ which appears to stretch the polymer and diminishes the probability for an entangled polymer with a high winding number n. This stretching potential may provide some insights into the still unsolved problem of protein folding and unfolding. In the following section, we present the application of white noise calculus to the one-dimensional random walk. This is followed by the entangled polymer viewed as a two-dimensional random walk on a plane in section 3.

2. Probability function and white noise analysis

To illustrate the use of white noise calculus [6–9] in evaluating the probability function, we consider here the one-dimensional random walk problem. We begin with the Wiener representation of the random walk along the x-axis which starts at x_0 and ends at x_1 given by

$$P(x_1, x_0; L) = \int \exp\left[-\frac{1}{2l}\int_0^L \left(\frac{\mathrm{d}x}{\mathrm{d}s}\right)^2 \mathrm{d}s\right] \mathcal{D}[x]. \tag{2.1}$$

In this probability function, each step is denoted by l and the total number of steps N is such that $Nl = L$. The probability function equation (2.1) can be cast in the language of white noise [9] by parametrizing the paths as

$$\begin{aligned} x(L) &= x_0 + \sqrt{2l}B(L) \\ &= x_0 + \sqrt{2l}\int_0^L \omega(s)\mathrm{d}s \end{aligned} \tag{2.2}$$

where $B(s)$ is a Brownian motion parametrized by $s, 0 \leqslant s \leqslant L$, and $\omega = \mathrm{d}B/\mathrm{d}s$ is the corresponding white noise variable. With equation (2.2), the exponential in equation (2.1) becomes

$$\exp\left[-\frac{1}{2l}\int_0^L \left(\frac{\mathrm{d}x}{\mathrm{d}s}\right)^2 \mathrm{d}s\right] = \exp\left[-\int_0^L \omega(s)^2\,\mathrm{d}s\right] \tag{2.3}$$

where $(\mathrm{d}x/\mathrm{d}s) = \sqrt{2l}\omega$. Since the integrand in equation (2.1) is now expressed as a white noise functional, the integral over the paths $\mathcal{D}[x]$ becomes an integral over the Gaussian white noise measure $\mathrm{d}\mu(\omega)$. We note, however, that

$$\mathrm{d}\mu(\omega) = N_\omega \exp\left[-\frac{1}{2}\int_0^L \omega(s)^2\,\mathrm{d}s\right]\mathrm{d}^\infty\omega \tag{2.4}$$

where N_ω is a normalization factor and the exponential is responsible for the Gaussian fall-off. More appropriately, $\mathcal{D}[x]$ (where $\mathcal{D}[x] = \mathrm{d}^\infty x$, in the context of path integrals [12]) is replaced by, $N_\omega\,\mathrm{d}^\infty\omega = \exp\left[\frac{1}{2}\int \omega(s)^2\,\mathrm{d}s\right]\mathrm{d}\mu(\omega)$. Multiplying the exponential with $\mathrm{d}\mu(\omega)$, we are led to a modification of equation (2.3) and shall, therefore, consider the white noise functional,

$$\begin{aligned} I_0 &= N\exp\left(-\int_0^L \omega(s)^2\,\mathrm{d}s\right)\exp\left(\frac{1}{2}\int_0^L \omega(s)^2\,\mathrm{d}s\right) \\ &= N\exp\left(-\frac{1}{2}\int_0^L \omega(s)^2\,\mathrm{d}s\right) \end{aligned} \tag{2.5}$$

where N is an appropriate normalization factor. To incorporate the endpoint x_1, we use the Donsker delta function [6, 13] $\delta(x(L) - x_1)$, to pin down the paths $x(s)$, where $x(L)$ is given by equation (2.2). This, together with the white noise functional (2.5), enables us to write the probability function, equation (2.1), as

$$P(x_1, x_0; L) = N\int \exp\left(-\frac{1}{2}\int_0^L \omega(s)^2\,\mathrm{d}s\right)\delta\left(x_0 + \sqrt{2l}\int_0^L \omega(s)\,\mathrm{d}s - x_1\right)\mathrm{d}\mu(\omega). \tag{2.6}$$

To evaluate equation (2.6), we may use the Fourier representation of the δ-function, i.e.,

$$\begin{aligned} P(x_1, x_0; L) = {} & \frac{1}{2\pi}\int_{-\infty}^{+\infty}\mathrm{d}\lambda\exp[\mathrm{i}\lambda(x_0 - x_1)] \\ & \times N\int \exp\left(\mathrm{i}\lambda\sqrt{2l}\int_0^L \omega(s)\,\mathrm{d}s\right)\exp\left(-\frac{1}{2}\int_0^L \omega(s)^2\,\mathrm{d}s\right)\mathrm{d}\mu(\omega). \end{aligned} \tag{2.7}$$

The integration over $\mathrm{d}\mu(\omega)$ can be done by noting that, from white noise calculus [6–9], the T-transform of I_0, equation (2.5), is given by

$$\begin{aligned} T I_0(\xi) &= \int \exp\left(\mathrm{i}\int \omega\xi\,\mathrm{d}s\right) I_0(\omega)\,\mathrm{d}\mu(\omega) \\ &= \exp\left(-\frac{1}{4}\int_0^L \xi^2\,\mathrm{d}s\right) \end{aligned} \tag{2.8}$$

where the normalization is taken as $N^{-1} = \int \exp\left[-\frac{1}{2}\int \omega(s)^2\,\mathrm{d}s\right]\mathrm{d}\mu(\omega)$. If we let $\xi = \lambda\sqrt{2l}$ in equation (2.7), then the integration over $\mathrm{d}\mu(\omega)$ is just $T I_0(\xi)$, equation (2.8). The probability function, equation (2.7), therefore becomes

$$P(x_1, x_0; L) = \frac{1}{2\pi}\int_{-\infty}^{+\infty}\exp[-(lL/2)\lambda^2 + \mathrm{i}(x_0 - x_1)\lambda]\,\mathrm{d}\lambda. \tag{2.9}$$

What remains is a Gaussian integral over λ, and we obtain the result for a one-dimensional random walk starting from x_0 and ending at x_1 [14],

$$P(x_1, x_0; L) = \sqrt{1/2\pi Nl^2}\exp[-(1/2Nl^2)(x_0 - x_1)^2] \tag{2.10}$$

where $Nl = L$. In the following sections, we apply this white noise functional approach to evaluate the entanglement probabilities of polymers.

3. Entangled polymers

Let us consider two polymers, where one entangles around the other. We can take the first polymer to lie on a plane with endpoints at $\mathbf{r}_0$ and $\mathbf{r}_1$, and the second polymer modelled by a straight line perpendicular to the plane and intersecting the origin. The various ways in which the polymer on the plane entangles around the second polymer, whether clockwise or anticlockwise, give rise to an interesting problem with topological constraints [2]. We can view the different possible configurations of the polymer on the plane as the paths of a random walk starting at $\mathbf{r}_0$ and ending at $\mathbf{r}_1$ in the presence of a singularity at the origin where the second polymer is located. Employing the polar coordinates $\mathbf{r} = (r, \vartheta)$ for this problem, Edwards [2] used the Wiener representation of the random walk in which the probability is represented by

$$P(\mathbf{r}_1, \mathbf{r}_0) = \int \exp\left[-\frac{1}{l}\int_0^L (\mathrm{d}\mathbf{r}/\mathrm{d}s)^2\,\mathrm{d}s\right]\mathcal{D}^2[\mathbf{r}] \tag{3.1}$$

where the integral is taken over all paths $\mathbf{r}(s)$ such that $\mathbf{r}(0) = \mathbf{r}_0$ and $\mathbf{r}(L) = \mathbf{r}_1$. Here, we represent the polymer as consisting of N freely hinged individual molecules, each of length l such that $L = Nl$. In view of the point singularity, a set of topologically equivalent configurations can be characterized by a winding number n, where $n = 0, \pm1, \pm2, \ldots$, indicating the number of times the polymer turns around the singular point at the origin ($n \geqslant 0$ signifies n turns anticlockwise and $n \leqslant -1$ means $|n+1|$ turns clockwise). Since we are interested in the number of possible windings around the origin that the polymer on the plane undergoes, we can simplify the calculation by fixing the radial variable to $r = R$, i.e., $\mathbf{r} = (R, \vartheta)$, and use ϑ to track the number of turns, clockwise or anticlockwise, around the origin. We note that a fixed radial part describes the entanglement scenario in the low-temperature limit [5] for any polymer interaction potential $V(r)$ which has a minimum at some value $r = R$. In this case, equation (3.1) reduces to

$$P(\vartheta_1, \vartheta_0) = \int \exp\left[-\frac{1}{l}\int_0^L R^2\left(\frac{\mathrm{d}\vartheta}{\mathrm{d}s}\right)^2\mathrm{d}s\right]\mathcal{D}[R\,\mathrm{d}\vartheta] \tag{3.2}$$

where $\vartheta_1 = \vartheta(L)$ and $\vartheta_0 = \vartheta(0)$.

The integrand can be written as a white noise functional by parametrizing the variable ϑ as

$$\begin{aligned}\vartheta(L) &= \vartheta_0 + (\sqrt{l}/R)B(L)\\ &= \vartheta_0 + (\sqrt{l}/R)\int_0^L \omega(s)\,\mathrm{d}s\end{aligned} \tag{3.3}$$

where $\omega = \mathrm{d}B/\mathrm{d}s$ and $\omega(s)$ is a Gaussian random white noise variable with $B(s)$ being a Brownian motion parametrized by s. Noting that $\mathrm{d}\vartheta/\mathrm{d}s = (\sqrt{l}/R)\omega(s)$, the integrand in equation (3.2) becomes

$$\exp\left[-\frac{1}{l}\int R^2\left(\frac{\mathrm{d}\vartheta}{\mathrm{d}s}\right)^2\mathrm{d}s\right] = \exp\left[-\int \omega(s)^2\,\mathrm{d}s\right]. \tag{3.4}$$

Having expressed the integrand as a white noise functional, the integration over $\mathcal{D}[R\,\mathrm{d}\vartheta]$ becomes an integral over the Gaussian white noise measure, or more appropriately (as seen in the previous section) an integral over, $N_\omega\,\mathrm{d}^\infty\omega = \exp\left[\frac{1}{2}\int \omega(s)^2\,\mathrm{d}s\right]\mathrm{d}\mu(\omega)$. The exponential factor, together with the right-hand side of equation (3.4), yields the white noise functional I_0 given by equation (2.5). Since the initial point ϑ_0 has been fixed by the parametrization equation (3.3), we can fix the endpoint ϑ_1 by using the Donsker delta function, $\delta(\vartheta(L) - \vartheta_1)$,

where $\vartheta(L)$ is given by equation (3.3). However, note that the polymer can wind n times clockwise, or anticlockwise, around the origin, and to reflect these possibilities we use instead $\delta(\vartheta(L) - \vartheta_1 + 2\pi n)$, where $n = 0, \pm 1, \pm 2, \ldots$. Hence I_0, equation (2.5), together with this delta function leads us to the white noise functional,

$$\begin{aligned} I &= \sum_{n=-\infty}^{+\infty} I_0 \delta(\vartheta(L) - \vartheta_1 + 2\pi n) \\ &= \sum_{n=-\infty}^{+\infty} N \exp\left(-\frac{1}{2}\int_0^L \omega(s)^2 \,\mathrm{d}s\right) \delta\left(\vartheta_0 + (\sqrt{l}/R)\int_0^L \omega(s)\,\mathrm{d}s - \vartheta_1 + 2\pi n\right). \end{aligned} \tag{3.5}$$

Integrating over the white noise measure $\mathrm{d}\mu(\omega)$, the probability function, equation (3.2), can now be written as

$$P(\vartheta_1, \vartheta_0) = \int \sum_{n=-\infty}^{+\infty} I_0 \delta(\vartheta(L) - \vartheta_1 + 2\pi n)\,\mathrm{d}\mu(\omega). \tag{3.6}$$

To evaluate this expression, we write the Fourier representation of the δ-function,

$$\begin{aligned} P(\vartheta_1, \vartheta_0) = \frac{1}{2\pi} \sum_{n=-\infty}^{+\infty} \int \exp[\mathrm{i}\lambda(\vartheta_0 - \vartheta_1 + 2\pi n)] \\ \times \int \exp\left(\mathrm{i}\lambda(\sqrt{l}/R)\int_0^L \omega(s)\,\mathrm{d}s\right) I_0\,\mathrm{d}\mu(\omega)\,\mathrm{d}\lambda \end{aligned} \tag{3.7}$$

and note that the integration over $\mathrm{d}\mu(\omega)$ can be done using equation (2.8) with $\xi = \lambda\sqrt{l}/R$. We obtain

$$\begin{aligned} P(\vartheta_1, \vartheta_0) &= \frac{1}{2\pi} \sum_{n=-\infty}^{+\infty} \int \exp[\mathrm{i}\lambda(\vartheta_0 - \vartheta_1 + 2\pi n)] \exp(-\lambda^2 lL/4R^2)\,\mathrm{d}\lambda \\ &= \sum_{n=-\infty}^{+\infty} P_n. \end{aligned} \tag{3.8}$$

The P_n is the corresponding probability function for polymer configurations which entangle n times around the origin. The sum of all the P_n gives the total probability function. The remaining integral in P_n is a Gaussian integral over λ, i.e.,

$$\begin{aligned} P_n &= \frac{1}{2\pi} \int \exp[\mathrm{i}\lambda(\vartheta_0 - \vartheta_1 + 2\pi n) - \lambda^2(lL/4R^2)]\,\mathrm{d}\lambda \\ &= \sqrt{R^2/lL\pi}\,\exp[-(R^2/lL)(\vartheta_0 - \vartheta_1 + 2\pi n)^2]. \end{aligned} \tag{3.9}$$

From equation (3.8) we may also use Poisson's sum formula [15],

$$\frac{1}{2\pi} \sum_{n=-\infty}^{+\infty} \exp(\mathrm{i}n\phi) = \sum_{m=-\infty}^{+\infty} \delta(\phi + 2\pi m) \tag{3.10}$$

to obtain

$$\begin{aligned} P(\vartheta_1, \vartheta_0) &= \frac{1}{2\pi} \sum_{m=-\infty}^{+\infty} \int \delta(\lambda + m) \exp[\mathrm{i}\lambda(\vartheta_0 - \vartheta_1) - \lambda^2(lL/4R^2)]\,\mathrm{d}\lambda \\ &= \frac{1}{2\pi} \sum_{m=-\infty}^{+\infty} \exp[-\mathrm{i}m(\vartheta_0 - \vartheta_1) - m^2(lL/4R^2)]. \end{aligned} \tag{3.11}$$

For an entangled polymer with an arbitrary initial starting point we may set $\vartheta_0 = \vartheta_1$. From equations (3.9) and (3.11), the probability that the polymer winds n times can be calculated as

$$W(n) = P_n/P(L) = \frac{\sqrt{R^2/lL\pi}\exp[-(2\pi nR)^2/lL]}{\frac{1}{2\pi}\sum_{m=-\infty}^{+\infty}\exp[-m^2(lL/4R^2)]}. \tag{3.12}$$

For a very long polymer, $L = Nl \gg 1$, the dominant term in the denominator is that for $m = 0$, and hence,

$$W(n) \approx (R/l)\sqrt{4\pi/N}\exp(-4\pi^2 n^2 R^2/Nl^2). \tag{3.13}$$

This result agrees with that obtained by Wiegel [5] for entangled polymers where an interaction potential has a minimum at some value $r = R$.

4. Polymer with magnetic flux

Let us next consider the case where the straight polymer intersecting the origin of the plane is endowed with a magnetic flux confined along its length. We represent this situation by adding a potential, $V = q\mathbf{A}\cdot\dot{\mathbf{r}}$, to the probability function, equation (3.1), which describes the various configurations of the entangled polymer lying on the plane. Here, q is the net charge of each repeating unit of the polymer, and $\mathbf{A}$ is the vector potential. Incorporating this in equation (3.1), we have

$$P(\mathbf{r}_1, \mathbf{r}_0) = \int \exp\left[-\frac{1}{l}\int_0^L [(\mathrm{d}\mathbf{r}/\mathrm{d}s)^2 + lq\mathbf{A}\cdot\dot{\mathbf{r}}]\,\mathrm{d}s\right]\mathcal{D}^2[\mathbf{r}]. \tag{4.1}$$

In particular, the vector potential $\mathbf{A}$ can be written as

$$\mathbf{A} = (\Phi_0/2\pi)\nabla\vartheta \qquad (r > R_0) \tag{4.2}$$

where R_0 is the cross-sectional radius of the straight polymer at the origin and $\Phi_0 = \pi R_0^2 B$ is the non-vanishing magnetic flux along its length. Note that outside the straight polymer, $r > R_0$, the magnetic field is $B = \nabla\times\mathbf{A} = 0$, which is a situation analogous to the Aharonov–Bohm set-up [10, 11]. With equation (4.2), the potential becomes $q\mathbf{A}\cdot\dot{\mathbf{r}} = \Phi\dot{\vartheta}$, where $\Phi = q\Phi_0/2\pi$, and equation (4.1) can be written as

$$P(\mathbf{r}_1, \mathbf{r}_0) = \int \exp\left[-\frac{1}{l}\int_0^L [(\mathrm{d}\mathbf{r}/\mathrm{d}s)^2 + l\Phi\dot{\vartheta}]\,\mathrm{d}s\right]\mathcal{D}^2[\mathbf{r}]. \tag{4.3}$$

As in the previous section, if we simplify the calculation by constraining the radial part to $r = R > R_0$, equation (4.3) becomes

$$P(\vartheta_1, \vartheta_0) = \int \exp\left[-\frac{1}{l}\int_0^L \left[R^2\left(\frac{\mathrm{d}\vartheta}{\mathrm{d}s}\right)^2 + l\Phi\dot{\vartheta}\right]\mathrm{d}s\right]\mathcal{D}[R\,\mathrm{d}\vartheta]. \tag{4.4}$$

Parametrizing the variable ϑ as in equation (3.3), the integrand of equation (4.4) can be written as a white noise functional and the probability function acquires a form similar to equation (3.6) modified by the potential, $\Phi\dot{\vartheta} = \Phi(\sqrt{l}/R)\omega$, i.e.,

$$P(\vartheta_1, \vartheta_0) = \int \sum_{n=-\infty}^{+\infty} I_0 \exp\left(-\Phi(\sqrt{l}/R)\int_0^L \omega(s)\,\mathrm{d}s\right) \times \delta\left(\vartheta_0 + (\sqrt{l}/R)\int_0^L \omega(s)\,\mathrm{d}s - \vartheta_1 + 2\pi n\right)\mathrm{d}\mu(\omega). \tag{4.5}$$

To facilitate the integration over $\mathrm{d}\mu(\omega)$, we use the Fourier representation of the delta function and write equation (4.5) as

$$P(\vartheta_1,\vartheta_0)=\frac{1}{2\pi}\sum_{n=-\infty}^{+\infty}\int_{-\infty}^{+\infty}\exp[\mathrm{i}\lambda(\vartheta_0-\vartheta_1+2\pi n)]\times\int\exp\left[\mathrm{i}(\sqrt{l}/R)(\lambda+\mathrm{i}\Phi)\int_0^L\omega(s)\,\mathrm{d}s\right]I_0\,\mathrm{d}\mu(\omega)\,\mathrm{d}\lambda. \tag{4.6}$$

If we let $\xi=(\sqrt{l}/R)(\lambda+\mathrm{i}\Phi)$, the integration over $\mathrm{d}\mu(\omega)$ is just the T-transform of I_0, equation (2.8), and the probability function becomes

$$P(\vartheta_1,\vartheta_0)\sum_{n=-\infty}^{+\infty}\frac{1}{2\pi}\int_{-\infty}^{+\infty}\exp[\mathrm{i}\lambda(\vartheta_0-\vartheta_1+2\pi n)]\exp[-(lL/4R^2)(\lambda+\mathrm{i}\Phi)^2]\,\mathrm{d}\lambda. \tag{4.7}$$

The remaining integral is a Gaussian integral over λ and we may write equation (4.7) as

$$P(\vartheta_1,\vartheta_0)=\sum_{n=-\infty}^{+\infty}P_n \tag{4.8}$$

where the probability for winding n times is given by

$$P_n=\sqrt{R^2/\pi lL}\exp\{-(R^2/lL)[\vartheta_0-\vartheta_1+2\pi n-(lL\Phi/2R^2)]^2\}\exp(lL\Phi^2/4R^2). \tag{4.9}$$

Alternatively, from equation (4.7), we may apply the Poisson sum formula, equation (3.10), such that

$$P(\vartheta_1,\vartheta_0)=\sum_{m=-\infty}^{+\infty}\frac{1}{2\pi}\int_{-\infty}^{+\infty}\delta(\lambda+m)\exp[\mathrm{i}\lambda(\vartheta_0-\vartheta_1)]\exp[-(lL/4R^2)(\lambda+\mathrm{i}\Phi)^2]\,\mathrm{d}\lambda \tag{4.10}$$

and integrate λ with the help of the delta function to obtain

$$P(\vartheta_1,\vartheta_0)=\frac{1}{2\pi}\sum_{m=-\infty}^{+\infty}\exp[-\mathrm{i}m(\vartheta_0-\vartheta_1-(\Phi lL/2R^2))]\exp[-(m^2lL/4R^2)+(lL\Phi^2/4R^2)]. \tag{4.11}$$

For the case when the flux $\Phi=0$, equation (4.11) reduces to equation (3.11).

The probability for the polymer to entangle n times is given by

$$W(n)=P_n/P(\vartheta_1,\vartheta_0)=\frac{\sqrt{R^2/lL\pi}\exp\{-(R^2/lL)[\vartheta_0-\vartheta_1+2\pi n-(Ll\Phi/2R^2)]^2\}}{\frac{1}{2\pi}\sum_{m=-\infty}^{+\infty}\exp\{-\mathrm{i}m[\vartheta_0-\vartheta_1-(\Phi lL/2R^2)]-m^2(lL/4R^2)\}}. \tag{4.12}$$

For an arbitrary initial point we may set $\vartheta_0=\vartheta_1$, and equation (4.12) may be written as

$$W(n)=\frac{R}{l}\sqrt{\frac{4\pi}{N}}\frac{\exp(-4\pi^2n^2R^2/Nl^2)\exp[2\pi n\Phi-(lL/4R^2)\Phi^2]}{\theta_3(\Phi Nl^2/4R^2)} \tag{4.13}$$

where $\theta_3(u)$ is the theta function [16],

$$\theta_3(u)=\sum_{m=-\infty}^{+\infty}q^{m^2}\exp(2mu\mathrm{i})=1+2\sum_{m=1}^{+\infty}q^{m^2}\cos(2mu) \tag{4.14}$$

with $u = \Phi Nl^2/4R^2$ and $q = \exp(-Nl^2/4R^2)$. For a very long polymer, $L = Nl \gg 1$, the $\theta_3(u)$ in the denominator is approximately 1, and we obtain from equation (4.13)

$$W(n) \approx (R/l)\sqrt{4\pi/N}\exp\{-(1/Nl^2)[2\pi nR - (Nl^2/2R)\Phi]^2\}. \tag{4.15}$$

Curiously, even if the magnetic flux Φ is confined along the straight polymer such that $B = 0$ in the region where the entangled polymer lies on the plane, the entanglement probability is still affected by the confined magnetic field. This is reminiscent of the Aharonov–Bohm effect in quantum mechanics [10, 11] where the interference pattern of the electron in a two-slit experiment is influenced by a magnetic field it never comes in contact with. Here, of course, we are dealing with 'classical' entanglement probabilities of a polymer which lies in a region where the force due to the confined magnetic field B is zero, and yet is still influenced by it. When the magnetic flux vanishes, $\Phi = 0$, the entanglement probability equation (4.15) reduces to equation (3.13), or equation (1.1) obtained by Wiegel.

5. Polymer with a $V = \dot{f}(s)\vartheta$ potential

Let us next consider the case where the polymer on the plane is subjected to a potential $V = \dot{f}(s)\vartheta$, as it entangles around the second straight polymer perpendicular to the plane at the origin. Here, $\dot{f} = \mathrm{d}f/\mathrm{d}s$, and we introduce the potential by adding it to the 'kinetic part' of equation (3.2) such that

$$P_V(\vartheta_1, \vartheta_0) = \int \exp\left\{-\frac{1}{l}\int_0^L \left[R^2\left(\frac{\mathrm{d}\vartheta}{\mathrm{d}s}\right)^2 + l\dot{f}(s)\vartheta\right]\mathrm{d}s\right\}\mathcal{D}[R\,\mathrm{d}\vartheta]. \tag{5.1}$$

We note that the potential part can also be written as

$$\begin{aligned}\int_0^L \frac{\mathrm{d}f}{\mathrm{d}s}\vartheta\,\mathrm{d}s &= \int_0^L \frac{\mathrm{d}}{\mathrm{d}s}(f\vartheta)\,\mathrm{d}s - \int_0^L f\left(\frac{\mathrm{d}\vartheta}{\mathrm{d}s}\right)\mathrm{d}s \\ &= f(L)\vartheta(L) - f(0)\vartheta(0) - \int_0^L f\dot{\vartheta}\,\mathrm{d}s \end{aligned} \tag{5.2}$$

where $f(L)$, $f(0)$, $\vartheta(L)$ and $\vartheta(0)$ are constants being values of the variables at the endpoints. Equation (5.2) allows us to write equation (5.1) as

$$\begin{aligned}P_V(\vartheta_1, \vartheta_0) &= \exp[f(0)\vartheta(0) - f(L)\vartheta(L)] \\ &\quad\times \int \exp\left\{-\frac{1}{l}\int_0^L \left[R^2\left(\frac{\mathrm{d}\vartheta}{\mathrm{d}s}\right)^2 - lf\dot{\vartheta}\right]\mathrm{d}s\right\}\mathcal{D}[R\,\mathrm{d}\vartheta].\end{aligned} \tag{5.3}$$

Parametrizing the variable ϑ as in equation (3.3), the integrand can be expressed as a white noise functional and the probability function $P_V(\vartheta_1, \vartheta_0)$ for the entangled polymer acquires the form of equation (3.6), but modified by the potential term (5.2) where we write $f\dot{\vartheta} = f(\sqrt{l}/R)\omega$, i.e.,

$$\begin{aligned}P_V(\vartheta_1, \vartheta_0) &= \exp[f(0)\vartheta(0) - f(L)\vartheta(L)] \\ &\quad\times \int \sum_{n=-\infty}^{+\infty} I_0 \exp\left[(\sqrt{l}/R)\int_0^L f\omega(s)\,\mathrm{d}s\right]\delta(\vartheta(L) - \vartheta_1 + 2\pi n)\,\mathrm{d}\mu(\omega).\end{aligned} \tag{5.4}$$

We again express the delta function in terms of its Fourier representation and obtain

$$\begin{aligned}P_V(\vartheta_1, \vartheta_0) &= \exp[f(0)\vartheta(0) - f(L)\vartheta(L)]\frac{1}{2\pi}\sum_{n=-\infty}^{+\infty}\int_{-\infty}^{+\infty}\exp[\mathrm{i}\lambda(\vartheta_0 - \vartheta_1 + 2\pi n)] \\ &\quad\times \int \exp\left\{\mathrm{i}\int_0^L (\sqrt{l}/R)(\lambda - \mathrm{i}f)\omega(s)\,\mathrm{d}s\right\} I_0\,\mathrm{d}\mu(\omega)\,\mathrm{d}\lambda.\end{aligned} \tag{5.5}$$

If we let $\xi = (\sqrt{l}/R)(\lambda - \mathrm{i}f)$, the integration over $\mathrm{d}\mu(\omega)$ is just the T-transform of I_0, equation (2.8). This yields

$$\begin{aligned} P_V(\vartheta_1, \vartheta_0) &= \exp[f(0)\vartheta(0) - f(L)\vartheta(L)]\frac{1}{2\pi}\sum_{n=-\infty}^{+\infty}\int_{-\infty}^{+\infty}\exp[\mathrm{i}\lambda(\vartheta_0 - \vartheta_1 + 2\pi n)] \\ &\quad \times \exp\left\{-(l/4R^2)\int_0^L(\lambda - \mathrm{i}f)^2\,\mathrm{d}s\right\}\mathrm{d}\lambda \\ &= \sum_{n=-\infty}^{+\infty} P_n \end{aligned} \tag{5.6}$$

where the Gaussian integral over λ in P_n can be evaluated to give

$$\begin{aligned} P_n = \sqrt{\frac{R^2}{\pi l L}}\exp[f(0)\vartheta(0) - f(L)\vartheta(L)]\exp\left[\left(\frac{l}{4R^2}\int_0^L f^2\,\mathrm{d}s\right)\right] \\ \times \exp\left[-\frac{R^2}{lL}\left(\vartheta_0 - \vartheta_1 + 2\pi n + \frac{l}{2R^2}\int_0^L f\,\mathrm{d}s\right)^2\right]. \end{aligned} \tag{5.7}$$

From equation (5.6), we can also employ the Poisson sum formula, equation (3.10), and integrate λ to obtain

$$\begin{aligned} P_V(\vartheta_1, \vartheta_0) = \frac{1}{2\pi}\exp[f(0)\vartheta(0) - f(L)\vartheta(L)]\sum_{m=-\infty}^{+\infty}\exp[-\mathrm{i}m(\vartheta_0 - \vartheta_1)] \\ \times \exp\left\{-\frac{m^2 lL}{4R^2} - \frac{\mathrm{i}ml}{2R^2}\int_0^L f\,\mathrm{d}s + \frac{l}{4R^2}\int_0^L f^2\,\mathrm{d}s\right\}. \end{aligned} \tag{5.8}$$

The probability that the polymer entangles n times can be obtained from equations (5.7) and (5.8) to yield (setting $\vartheta_0 = \vartheta_1$)

$$\begin{aligned} W(n) &= P_n/P_V \\ &= \frac{R}{l}\sqrt{\frac{4\pi}{N}}\,\frac{\exp\left[-\frac{R^2}{Nl^2}\left(2\pi n + \frac{l}{2R^2}\int_0^L f\,\mathrm{d}s\right)^2\right]}{\theta_3\left(\frac{l}{4R^2}\int_0^L f\,\mathrm{d}s\right)} \end{aligned} \tag{5.9}$$

where $\theta_3(u)$ is the theta function, equation (4.14), with $u = (l/4R^2)\int f\,\mathrm{d}s$, and $q = \exp(-Nl^2/4R^2)$.

As an example, let us consider the potential $V = k\vartheta$ (k is constant), which could be obtained from $V = \dot{f}(s)\vartheta$, if we let $f = ks$. In this case, the probability for n entanglements, equation (5.9), becomes

$$W(n) = \frac{R}{l}\sqrt{\frac{4\pi}{N}}\,\frac{\exp\left[-\frac{R^2}{Nl^2}\left(2\pi n + \frac{kL^2 l}{4R^2}\right)^2\right]}{1 + 2\sum_{m=-\infty}^{+\infty}\exp(-m^2 Nl^2/4R^2)\cos(mkL^2 l/4R^2)}. \tag{5.10}$$

For a very long macromolecule, $L = Nl \gg 1$, the denominator is approximately 1 and we have

$$W(n) \approx \frac{R}{l}\sqrt{\frac{4\pi}{N}}\exp(-4\pi^2 n^2 R^2/Nl^2)\exp[-nkNl\pi - (k^2 N^3 l^4/16R^2)]. \tag{5.11}$$

For $k = 0$, we recover the previous result, equation (1.1) or (3.13). The effect of the potential $V = k\vartheta$, as exhibited by the appearance of the second exponential factor in $W(n)$, is to greatly diminish the probability for higher winding numbers n. This $V = k\vartheta$ inhibits the coiling of the polymer on the plane and acts like a stretching potential.

6. Conclusion

Using white noise analysis, we extend the study of two chainlike macromolecules and their entanglement by considering two types of potential: (a) a magnetic flux confined along the straight polymer perpendicular to the plane, and (b) a $V = \dot{f}(s)\vartheta$ potential to which the entangled polymer is subjected on the plane. The probability $W(n)$ for the polymer on the plane to entangle n times around the straight polymer is calculated for both types of potential. When the potentials considered are taken to be zero, we obtain the $W(n)$ previously derived by Wiegel [5].

The case involving a magnetic flux confined along the straight polymer appears to be a classical analogue of the Aharonov–Bohm effect in quantum mechanics. The entanglement probability $W(n)$ is influenced by the magnetic flux, even if the entangled polymer lies in a region where $B = 0$, and feels no magnetic force. It would be interesting to see whether an experimental observation of this effect could be realized with the development of insulated molecular wires made from a conducting linear polymer covered with a molecular nanotube that acts as an insulator [17].

The potential $V = \dot{f}(s)\vartheta$, on the other hand, appears to stretch the polymer and leads to a $W(n)$ which shows a further decrease in the probability for a large winding number n to occur. This type of stretching potential may be useful in understanding how a long macromolecule, such as a protein, coils and uncoils as it adopts a stable configuration.

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References

[1] Bernido C C and Carpio-Bernido M V 2002 Path integrals for boundaries and topological constraints: a white noise functional approach *J. Math. Phys.* **43** 1728–36
[2] Edwards S F 1967 Statistical mechanics with topological constraints: I *Proc. Phys. Soc. Lond.* **91** 513–9
[3] Prager S and Frisch H L 1967 *J. Chem. Phys.* **46** 1475
[4] Saito N and Chen Y 1973 *J. Chem. Phys.* **59** 3701
[5] Wiegel F W 1977 Entanglement probabilities for a harmonically bound macromolecule *J. Chem. Phys.* **67** 469–72
[6] Hida T, Kuo H H, Potthoff J and Streit L 1993 *White Noise. An Infinite Dimensional Calculus* (Dordrecht: Kluwer)
[7] Obata N 1994 *White Noise Calculus and Fock Space (Lecture Notes in Mathematics vol 1577)* (Berlin: Springer)
[8] Kuo H H 1996 *White Noise Distribution Theory* (Boca Raton, FL: CRC Press)
[9] For the quantum propagator, see, e.g., Streit L and Hida T 1983 Generalized Brownian functionals and the Feynman integral *Stoch. Process. Appl.* **16** 55–69
[10] Peshkin M and Tonomura A 1989 *The Aharonov–Bohm Effect* (Berlin: Springer)

[11] See, e.g., Bernido C C and Inomata A 1981 Path integrals with a periodic constraint: the Aharonov–Bohm effect *J. Math. Phys.* **22** 715
[12] Feynman R P and Hibbs A R 1965 *Quantum Mechanics and Path Integrals* (New York: McGraw-Hill)
[13] Lascheck A, Leukert P, Streit L and Westerkamp W 1994 More about Donsker's delta function *Soochow J. Math.* **20** 401–18
[14] See, e.g., Chandrasekhar S 1943 Stochastic problems in physics and astronomy *Rev. Mod. Phys.* **15** 1–89
[15] Bellman R 1961 *A Brief Introduction to Theta Functions* (New York: Holt, Rinehart and Winston)
[16] Gradshteyn I S and Ryzhik I M 1994 *Table of Integrals, Series, and Products* 5th edn (San Diego, CA: Academic) p 927
[17] See, e.g., Shimomura T, Akai T, Abe T and Ito K 2002 Atomic force microscopy observation of insulated molecular wire formed by conducting polymer and molecular nanotube *J. Chem. Phys.* **116** 1753–6