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ENTITLED SEGMENT DENSITY FUNCTIONS OF POLYMER CHAINS

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ABSTRACT

A theoretical investigation into the segment density profile of confined chains has been undertaken herein, where the confinement is between a pair of infinite parallel walls which are reflecting or absorbing. Exact infinite series expressions are derived for the segment density functions of cilia, loops, bridges, and floating chains. These infinite series are easily evaluated numerically.

1. INTRODUCTION

A great many theoretical problems in polymer physics are concerned with the behavior of polymer chains in the presence of surfaces.^[1] In previous studies, the conformational statistics of these confined chains have been calculated either by using the method of images or by solving the diffusion equation, both reflecting and absorbing boundary conditions have been used in these studies. The case of the polymer chain in the presence of a single wall, the "one-wall" problem, yields simple analytical results. The case of the chain between two parallel walls, the "two-wall" problem, results in infinite series expressions which require a computer in order to be evaluated (see Appendix for program flowcharts and listing).

In this thesis, we will derive the segment density functions of an individual polymer chain between two infinite parallel walls which are (i) reflecting or (ii) absorbing. We consider a loop (a chain with both ends attached to one wall), a bridge (a chain with each end attached to a different wall), a cilium (a chain with one end attached to a wall and one unattached end) and a floating chain (a chain which is attached to neither wall). We will obtain exact infinite series expressions which can be well approximated by their leading terms for various values of wall separation.

2. GENERAL FORMS FOR THE CONFINED CHAIN DISTRIBUTION FUNCTIONS

The end-to-end distribution function for a polymer chain consisting of N segments and having its ends located at (x_A, y_A, z_A) and (x_B, y_B, z_B) can be written in the Gaussian approximation as: [2]

$$\begin{aligned}
 W(x_A, y_A, z_A; x_B, y_B, z_B; N) = & \{(\beta_N/\pi)^{1/2} \exp[-\beta_N(x_A - x_B)^2]\} \\
 & \cdot \{(\beta_N/\pi)^{1/2} \exp[-\beta_N(y_A - y_B)^2]\} \\
 & \cdot \{(\beta_N/\pi)^{1/2} \exp[-\beta_N(z_A - z_B)^2]\}
 \end{aligned}
 \tag{1}$$

where $\beta_N = (3/2\langle r^2 \rangle_*)$. The quantity $\langle r^2 \rangle_*$ represents that portion of the mean square end-to-end separation of the unperturbed chain which is directly proportional to N . The chain distribution function given in Eq. (1) is spherically symmetric. It is applicable to a polymer chain with short-range interactions such as fixed valence angle and hindered internal rotation and no long-range excluded volume interactions.

If we now confine the polymer chain between two barriers, a distance d apart, using the $x = 0$ and $x = d$ planes, we can write the confined chain distribution function for the cases where (i) the barriers are reflecting and (ii) the barriers are absorbing, as:

$$\begin{aligned}
W_{\text{absorbing}}(x_A; x_B; N; d) = & (\beta_N/\pi)^{1/2} \sum_{m=-\infty}^{\infty} \{ \exp[-\beta_N(x_A - x_B \\
& - 2md)^2] - \exp[-\beta_N(x_A + x_B \\
& - 2md)^2] \} \quad (2)
\end{aligned}$$

$$\begin{aligned}
W_{\text{reflecting}}(x_A; x_B; N; d) = & (\beta_N/\pi)^{1/2} \sum_{m=-\infty}^{\infty} \{ \exp[-\beta_N(x_A - x_B \\
& - 2md)^2] + \exp[-\beta_N(x_A + x_B \\
& - 2md)^2] \} \quad (3)
\end{aligned}$$

Equations (2) and (3) are obtained by using the method of images^[3-5] (which is valid only for symmetric, non-self-avoiding random walks) and integrating Eq. (1) over its y and z components.

We can use Equations (2) and (3) to develop two equivalent infinite series expressions for each confined chain distribution function. One expression, denoted by the subscript "*small*", can be well approximated by the leading terms in the infinite series at small values of d while the other expression, denoted by the subscript "*large*", can be well approximated by the leading terms in the infinite series at large values of d .

Small Wall Forms

According to the theorem of Carslaw and Jaeger,^[6] if $f(x)$ is an even function in x , then

$$\begin{aligned}
\sum_{m=-\infty}^{\infty} f(x - 2md) &= (1/d) \int_0^{\infty} f(x') dx' + (2/d) \\
&\cdot \sum_{m=-\infty}^{\infty} \cos(m\pi x/d) \\
&\cdot \int_0^{\infty} f(x') \cos(m\pi x'/d) dx' \quad (4)
\end{aligned}$$

Using this theorem, we derive

$$\begin{aligned}
\sum_{m=-\infty}^{\infty} \left\{ \left(\frac{\beta_N}{\pi} \right)^{1/2} \exp[-\beta_N (x_A \pm x_B - 2md)^2] \right\} &= \frac{1}{2d} + \frac{1}{d} \\
&\cdot \sum_{m=-\infty}^{\infty} \left[\exp\left(-\frac{m^2 \pi^2}{4\beta_N d^2}\right) \right] \\
&\cdot \left[\cos\left(\frac{m\pi x_A}{d}\right) \cos\left(\frac{m\pi x_B}{d}\right) \right. \\
&\left. \pm \sin\left(\frac{m\pi x_A}{d}\right) \sin\left(\frac{m\pi x_B}{d}\right) \right] \quad (5)
\end{aligned}$$

Substituting this result into Equations (2) and (3) yields

$$\begin{aligned}
W_{\substack{\text{absorbing} \\ \text{small}}} (x_A; x_B; N; d) &= \frac{2}{d} \sum_{m=1}^{\infty} \left[\exp\left(-\frac{m^2 \pi^2}{4\beta_N d^2}\right) \right] \\
&\cdot \left[\sin\left(\frac{m\pi x_A}{d}\right) \sin\left(\frac{m\pi x_B}{d}\right) \right] \quad (6)
\end{aligned}$$

$$W_{\text{reflecting}}^{\text{small}}(x_A; x_B; N; d) = \frac{1}{d} + \frac{2}{d} \sum_{m=1}^{\infty} \left[\exp\left(-\frac{m^2 \pi^2}{4\beta_N d^2}\right) \right] \cdot \left[\cos\left(\frac{m\pi x_A}{d}\right) \cos\left(\frac{m\pi x_B}{d}\right) \right] \quad (7)$$

Large Wall Forms

In general, we will use the same expressions, given in Equations (2) and (3)

$$W_{\text{absorbing}}^{\text{large}}(x_A; x_B; N; d) = \left(\frac{\beta_N}{\pi}\right)^{\frac{1}{2}} \sum_{m=-\infty}^{\infty} \left\{ \exp[-\beta_N (x_A - x_B - 2md)^2] - \exp[(x_A + x_B - 2md)^2] \right\} \quad (8)$$

$$W_{\text{reflecting}}^{\text{large}}(x_A; x_B; N; d) = \left(\frac{\beta_N}{\pi}\right)^{\frac{1}{2}} \sum_{m=-\infty}^{\infty} \left\{ \exp[-\beta_N (x_A - x_B - 2md)^2] + \exp[-\beta_N (x_A + x_B - 2md)^2] \right\} \quad (9)$$

When one end of the chain, x_B , is fixed at a very small distance, λ , away from the $x = 0$ plane, we can use the approximations $\exp(-\beta_N \lambda^2) \approx 1$ and $\exp[\pm 2\beta_N \lambda (x_A - 2md)] \approx 1 \pm [2\beta_N \lambda \cdot (x_A - 2md)]$ in Equations (8) and (9) to obtain

$$\begin{aligned}
W_{\substack{\text{absorbing} \\ \text{large}}} (x_A; x_B = \lambda; N; d) &= \left(\frac{\beta_N}{\pi} \right)^{\frac{1}{2}} (4\beta_N \lambda) \sum_{m=-\infty}^{\infty} \{ (x_A - 2md) \\
&\quad \cdot \exp[-\beta_N (x_A - 2md)^2] \} \\
&= \left[\left(\frac{\beta_N}{\pi} \right)^{\frac{1}{2}} (4\beta_N \lambda) \right] \{ x_A \exp(-\beta_N x_A^2) \\
&\quad + \sum_{m=1}^{\infty} (x_A + 2md) \exp[-\beta_N (x_A + 2md)^2] \\
&\quad - \sum_{m=1}^{\infty} (2md - x_A) \exp[-\beta_N (2md - x_A)^2] \} \\
&\hspace{15em} (10)
\end{aligned}$$

$$\begin{aligned}
W_{\substack{\text{reflecting} \\ \text{large}}} (x_A; x_B = \lambda; N; d) &= \left(\frac{4\beta_N}{\pi} \right)^{\frac{1}{2}} \sum_{m=-\infty}^{\infty} \exp[-\beta_N (x_A - 2md)^2] \\
&= \left(\frac{4\beta_N}{\pi} \right)^{\frac{1}{2}} \{ \exp(-\beta_N x_A^2) \\
&\quad + \sum_{m=1}^{\infty} \exp[-\beta_N (x_A + 2md)^2] \\
&\quad + \sum_{m=1}^{\infty} \exp[-\beta_N (2md - x_A)^2] \} \\
&\hspace{15em} (11)
\end{aligned}$$

3. THE CHAIN DISTRIBUTION FUNCTIONS FOR A LOOP, CILIAM, FLOATING CHAIN AND BRIDGE

The calculation of the chain distribution functions of the various types of confined chains is performed using the following relationships:

$$W_{bridge} = W(x_A = d - \lambda; x_B = \lambda; N; d) \quad (12)$$

$$W_{loop} = W(x_A = \lambda; x_B = \lambda; N; d) \quad (13)$$

$$\begin{aligned} W_{cilium} &= W(0 < x_A < d; x_B = \lambda; N; d) \\ &= \int_0^d dx_A W(x_A; x_B = \lambda; N; d) \end{aligned} \quad (14)$$

$$\begin{aligned} W_{floating\ chain} &= W(0 < x_A < d; 0 < x_B < d; N; d) \\ &= \left(\frac{1}{d}\right) \int_0^d dx_B \int_0^d dx_A W(x_A; x_B; N; d) \end{aligned} \quad (15)$$

After substituting Equations (6)-(11) into these formulas and using the approximations: $\sin(m\pi\lambda/d) \approx (m\pi\lambda/d)$, $\sin[m\pi(d - \lambda)]/d \approx (-1)^{m+1}(m\pi\lambda)/d$, $\cos(m\pi\lambda)/d \approx 1$, $\cos[m\pi(d - \lambda)]/d \approx (-1)^m$, $\exp(\pm 4\beta_N \lambda m d) \approx 1 \pm (4\beta_N \lambda m d)$, $\exp(-\beta_N \lambda^2) \approx 1$, $\exp[\pm 2\beta_N d \lambda (2m - 1)] \approx 1 \pm [2\beta_N d \lambda (2m - 1)]$, the calculations are straightforward. The results are given in Equations (16)-(29) (beneath each equation the range is given in which the

infinite series expression can be approximated by its $m=1$ term to better than 95% accuracy, using the criterion that the second term is less than five percent of the first term in magnitude):

$$W_{\text{bridge absorbing small}} = \frac{2\pi^2\lambda^2}{d^3} \sum_{m=1}^{\infty} (-1)^{m+1} m^2 \exp\left(-\frac{m^2\pi^2}{4\beta_N d^2}\right) \quad (\beta_N^{1/2}d) < 1.3 \quad (16)$$

$$W_{\text{bridge absorbing large}} = \left(\frac{\beta_N}{\pi}\right)^{1/2} (8\beta_N\lambda^2) \sum_{m=1}^{\infty} \left\{ \exp[-(2m-1)^2] \cdot \beta_N d^2 \right\} \cdot [2\beta_N(2m-1)^2 d^2 - 1] \quad (\beta_N^{1/2}d) > 0.9 \quad (17)$$

$$W_{\text{loop absorbing small}} = \left(\frac{2\pi^2\lambda^2}{d^3}\right) \sum_{m=1}^{\infty} m^2 \exp\left(-\frac{m^2\pi^2}{4\beta_N d^2}\right) \quad (\beta_N^{1/2}d) < 1.3 \quad (18)$$

$$W_{\text{loop absorbing large}} = (4\beta_N^2\lambda^2) \left(\frac{\beta_N}{\pi}\right)^{1/2} \left\{ 1 + 2 \sum_{m=1}^{\infty} [\exp(-4m^2\beta_N d^2) \cdot (1 - 8m^2\beta_N d^2)] \right\} \quad (\beta_N^{1/2}d) > 0.7 \quad (19)$$

$$W_{\text{cilium absorbing small}} = \left(\frac{4\lambda}{d}\right) \sum_{m=1}^{\infty} \exp\left[-\frac{(2m-1)^2\pi^2}{4\beta_N d^2}\right] \quad (\beta_N^{1/2}d) < 2.5 \quad (20)$$

$$\begin{aligned}
 W_{\substack{\text{cilium} \\ \text{absorbing} \\ \text{large}}} &= 2\lambda \left(\frac{\beta_N}{\pi}\right)^{\frac{1}{2}} \left\{ 1 + 2 \sum_{m=1}^{\infty} (-1)^m \right. \\
 &\quad \cdot \left. \exp(-m^2 \beta_N d^2) \right\} \\
 &\quad (\beta_N^{\frac{1}{2}} d) > 1.0 \quad (21)
 \end{aligned}$$

$$\begin{aligned}
 W_{\substack{\text{floating chain} \\ \text{absorbing} \\ \text{small}}} &= \left(\frac{8}{\pi^2}\right) \sum_{m=1}^{\infty} (2m-1)^{-2} \\
 &\quad \cdot \exp\left[-\frac{(2m-1)^2 \pi^2}{4\beta_N d^2}\right] \\
 &\quad (\beta_N^{\frac{1}{2}} d) < 5.0 \quad (22)
 \end{aligned}$$

$$\begin{aligned}
 W_{\substack{\text{floating chain} \\ \text{absorbing} \\ \text{large}}} &= 1 + 4 \left[\sum_{m=1}^{\infty} m(-1)^m \operatorname{erfc}(m\beta_N^{\frac{1}{2}} d) \right] \\
 &\quad - 2(\beta_N \pi d^2)^{-\frac{1}{2}} - 4(\beta_N \pi d^2)^{\frac{1}{2}} \\
 &\quad \cdot \left\{ \sum_{m=1}^{\infty} (-1)^m \exp(-m^2 \beta_N d^2) \right\} \\
 &\quad (\beta_N^{\frac{1}{2}} d) > 1.0 \quad (23)
 \end{aligned}$$

$$\begin{aligned}
 W_{\substack{\text{bridge} \\ \text{reflecting} \\ \text{small}}} &= \frac{1}{d} + \frac{2}{d} \left\{ \sum_{m=1}^{\infty} (-1)^m \exp\left(-\frac{m^2 \pi^2}{4\beta_N d^2}\right) \right\} \\
 &\quad (\beta_N^{\frac{1}{2}} d) < 1.5 \quad (24)
 \end{aligned}$$

$$\begin{aligned}
 W_{\substack{\text{bridge} \\ \text{reflecting} \\ \text{large}}} &= 4 \left(\frac{\beta_N}{\pi}\right)^{\frac{1}{2}} \sum_{m=1}^{\infty} \left\{ \exp[-(2m-1)^2 \beta_N d^2] \right\} \\
 &\quad (\beta_N^{\frac{1}{2}} d) > 0.7 \quad (25)
 \end{aligned}$$

$$W_{\text{loop reflecting small}} = \frac{1}{d} + \frac{2}{d} \left\{ \sum_{m=1}^{\infty} \left[\exp\left(-\frac{m^2 \pi^2}{4\beta_N d^2}\right) \right] \right\} \quad (\beta_N^{1/2} d) < 1.5 \quad (26)$$

$$W_{\text{loop reflecting large}} = 2\left(\frac{\beta_N}{\pi}\right)^{1/2} \left\{ 1 + 2 \sum_{m=1}^{\infty} \left[\exp(-4m^2 \beta_N d^2) \right] \right\} \quad (\beta_N^{1/2} d) > 0.5 \quad (27)$$

$$W_{\text{cilium reflecting small}} = W_{\text{cilium reflecting large}} = 1 \quad (28)$$

$$W_{\text{floating chain reflecting small}} = W_{\text{floating chain reflecting large}} = 1 \quad (29)$$

These distribution functions are not normalized. The loop, cilium and floating chain normalized distribution functions are given by W/A where A is the $\lim_{d \rightarrow \infty} W_{\text{large}}$. The values of A are:

$$A_{\text{loop absorbing}} = (4\beta_N \lambda^2) \left(\frac{\beta_N}{\pi}\right)^{1/2} \quad (30)$$

$$A_{\text{loop reflecting}} = \left(\frac{4\beta_N}{\pi}\right)^{1/2} \quad (31)$$

$$A_{\text{cilium absorbing}} = \left(\frac{2\lambda\beta_N}{\pi}\right)^{1/2} \quad (32)$$

$$A_{\text{cilium reflecting}} = A_{\text{floating chain absorbing}} = A_{\text{floating chain reflecting}} = 1 \quad (33)$$

The bridge distribution function can not be normalized in this manner because A_{bridge} equals zero for the reflecting and absorbing wall cases.

4. SEGMENT DENSITY FUNCTIONS

The density distribution of chain segments for the various types of chains are calculated using the following relationships:

$$\begin{aligned} \rho_{cilium} = & \left(\frac{1}{N}\right) \int_0^N dk \{ [W(x_A=\xi; x_B=\lambda; k; d) \\ & \cdot W(x_A=\xi; 0 < x_B < d; N-k; d)] \cdot \left(\frac{1}{W_{cilium}}\right) \} \end{aligned} \quad (34)$$

$$\begin{aligned} \rho_{loop} = & \left(\frac{1}{N}\right) \int_0^N dk \{ [W(x_A=\xi; x_B=\lambda; k; d) \\ & \cdot W(x_A=\xi; x_B=\lambda; N-k; d)] \cdot \left(\frac{1}{W_{loop}}\right) \} \end{aligned} \quad (35)$$

$$\begin{aligned} \rho_{bridge} = & \left(\frac{1}{N}\right) \int_0^N dk \{ [W(x_A=\xi; x_B=\lambda; k; d) \\ & \cdot W(x_A=\xi; x_B=d-\lambda; N-k; d)] \cdot \left(\frac{1}{W_{bridge}}\right) \} \end{aligned} \quad (36)$$

$$\begin{aligned} \rho_{floating\ chain} = & \left(\frac{1}{N}\right) \int_0^N dk \{ [W(0 < x_A < d; x_B=\xi; k; d) \\ & \cdot \frac{W(x_A=\xi; 0 < x_B < d; N-k; d)}{W_{floating\ chain}}] \} \end{aligned} \quad (37)$$

There are three basic terms in these formulas:

$W(x_A=\lambda; x_B=\xi; t; d)$, $W(x_A=\xi; 0 < x_B < d; t; d)$ and $W(x_A=\xi; x_B=d-\lambda; t; d)$.

Using Equations (6)-(11) we can derive these terms for the various large and small wall forms:

$$W_{\substack{\text{absorbing} \\ \text{small}}}(x_A=\lambda; x_B=\xi; t; d) = \left(\frac{2\pi\lambda}{d^2}\right) \sum_{m=1}^{\infty} m \exp\left(-\frac{m^2\pi^2}{4\beta_t d^2}\right) \cdot \sin\left(\frac{m\pi\xi}{d}\right) \quad (38)$$

$$W_{\substack{\text{absorbing} \\ \text{small}}}(x_A=\xi; 0 < x_B < d; t; d) = \left(\frac{4}{\pi}\right) \sum_{m=1}^{\infty} (2m-1)^{-1} \cdot \exp\left[-\frac{(2m-1)^2\pi^2}{4\beta_t d^2}\right] \cdot \sin\left[\frac{(2m-1)\pi\xi}{d}\right] \quad (39)$$

$$W_{\substack{\text{absorbing} \\ \text{small}}}(x_A=\xi; x_B=d-\lambda; t; d) = \left(\frac{2\pi\lambda}{d^2}\right) \sum_{m=1}^{\infty} (-1)^{m+1} \cdot m \exp\left(-\frac{m^2\pi^2}{4\beta_t d^2}\right) \cdot \sin\left(\frac{m\pi\xi}{d}\right) \quad (40)$$

$$\begin{aligned}
W_{\text{absorbing}}^{(x_A=\lambda; x_B=\xi; t; d)}_{\text{large}} &= (4\lambda\beta_t) \left(\frac{\beta_t}{\pi}\right)^{\frac{1}{2}} \cdot \{\xi \exp(-\beta_t \xi^2) \\
&+ \sum_{m=1}^{\infty} (\xi + 2md) \\
&\cdot \exp[-\beta_t (\xi + 2md)^2] \\
&- \sum_{m=1}^{\infty} (2md - \xi) \\
&\cdot \exp[-\beta_t (2md - \xi)^2]\} \quad (41)
\end{aligned}$$

$$\begin{aligned}
W_{\text{absorbing}}^{(x_A=\xi; 0 < x_B < d; t; d)}_{\text{large}} &= \operatorname{erf}(\beta_t^{\frac{1}{2}} \xi) + \sum_{m=1}^{\infty} (-1)^m \\
&\cdot \operatorname{erf}[\beta_t^{\frac{1}{2}} (md + \xi)] \\
&- \sum_{m=1}^{\infty} (-1)^m \operatorname{erf}[\beta_t^{\frac{1}{2}} (md - \xi)] \quad (42)
\end{aligned}$$

$$\begin{aligned}
W_{\text{absorbing}}^{(x_A=\xi; x_B=d-\lambda; t; d)}_{\text{large}} &= (2\beta_t \lambda) \left(\frac{\beta_t}{\pi}\right)^{\frac{1}{2}} \left(\sum_{m=1}^{\infty} [(2m-1)d - \xi] \right. \\
&\cdot \exp\{-\beta_t [(2m-1)d - \xi]^2\} \\
&- \sum_{m=1}^{\infty} [\xi + (2m-1)d] \\
&\cdot \exp\{-\beta_t [\xi + (2m-1)d]^2\} \Bigg) \quad (43)
\end{aligned}$$

$$W_{\text{reflecting}}^{\text{small}}(x_A=\lambda; x_B=\xi; t; d) = \frac{1}{d} + \frac{2}{d} \sum_{m=1}^{\infty} \exp\left(-\frac{m^2 \pi^2}{4\beta_t d^2}\right) \cdot \cos\left(\frac{m\pi\xi}{d}\right) \quad (44)$$

$$W_{\text{reflecting}}^{\text{small}}(x_A=\xi; 0 < x_B < d; t; d) = 1 \quad (45)$$

$$W_{\text{reflecting}}^{\text{small}}(x_A=\xi; x_B=d-\lambda; t; d) = \frac{1}{d} + \frac{2}{d} \sum_{m=1}^{\infty} (-1)^m \exp\left(-\frac{m^2 \pi^2}{4\beta_t d^2}\right) \cdot \cos\left(\frac{m\pi\xi}{d}\right) \quad (46)$$

$$W_{\text{reflecting}}^{\text{large}}(x_A=\lambda; x_B=\xi; t; d) = \left(\frac{4\beta_t}{\pi}\right)^{\frac{1}{2}} \left\{ \exp(-\beta_t \xi^2) + \sum_{m=1}^{\infty} \exp[-\beta_t (\xi + 2md)^2] + \sum_{m=1}^{\infty} \exp[-\beta_t (2md - \xi)^2] \right\} \quad (47)$$

$$W_{\text{reflecting}}^{\text{large}}(x_A=\xi; 0 < x_B < d; t; d) = 1 \quad (48)$$

$$W_{\text{reflecting}}^{\text{large}}(x_A=\xi; x_B=d-\lambda; t; d) = \left(\frac{\beta_t}{\pi}\right)^{\frac{1}{2}} \left(\sum_{m=1}^{\infty} \exp\{-\beta_t [(2m-1)d - \xi]^2\} + \sum_{m=1}^{\infty} \exp\{-\beta_t [(2m-1)d - \xi]^2\} \right) \quad (49)$$

The calculation of the segment density functions using Equations (16) through (29), (34) through (37) and (38) through (49) is straightforward. In the small wall form case, the integration over k is done using the relation

$(\beta_k^{-1} + \beta_{N-k}^{-1} = \beta_N^{-1})$ and the following series summations^[7]

$$\sum_{\substack{m=1 \\ m \neq \ell}}^{\infty} (m^2 - \ell^2)^{-1} m \sin(mx) = \left[\left(\frac{\pi}{2} \right) - \left(\frac{x}{2} \right) \right] \cos(\ell x) - \left(\frac{1}{4\ell} \right) \sin(\ell x)$$

$$\sum_{m=1}^{\infty} m^{-2} \cos(mx) = \left(\frac{1}{12} \right) (3x^2 - 6\pi x + 2\pi^2)$$

$$\sum_{\substack{m=1 \\ m \neq \ell}}^{\infty} (m^2 - \ell^2)^{-1} \cos(mx) = \left(\frac{1}{4\ell^2} \right) [2 + \cos(\ell x) + 2\ell(x - \pi) \cdot \sin(\ell x)]$$

(50)

In the large wall form case, the integration over k is carried out using the Laplacian folding operation

$$\int_0^N dk [f(k)g(N-k)] = L^{-1}\{L[f(k)] \cdot L[g(N-k)]\} \quad (51)$$

where L is the Laplace transform and L^{-1} is the inverse Laplace transform. The expressions which are obtained for the segment density functions are:

$$\begin{aligned}
\rho_{\text{loop absorbing small}} &= \left[\left(\frac{2}{d} \right) \sum_{r=1}^{\infty} r^2 \sin^2 \left(\frac{r\pi\xi}{d} \right) \exp \left(- \frac{r^2 \pi^2}{4\beta_N d^2} \right) \right. \\
&+ \left(\frac{16\beta_N d}{\pi^2} \right) \sum_{n=1}^{\infty} n \sin \left(\frac{n\pi\xi}{d} \right) \exp \left(- \frac{\pi^2 n^2}{4\beta_N d^2} \right) \\
&\cdot \left\{ \left(\frac{\pi}{2} \right) \left[1 - \left(\frac{\xi}{d} \right) \right] \cos \left(\frac{n\pi\xi}{d} \right) - (4n)^{-1} \right. \\
&\cdot \left. \left. \sin \left(\frac{n\pi\xi}{d} \right) \right] \right\} \cdot \left\{ \left[\sum_{p=1}^{\infty} p^2 \exp \left(- \frac{p^2 \pi^2}{4\beta_N d^2} \right) \right] \right\}
\end{aligned} \tag{52}$$

$$\begin{aligned}
\rho_{\text{floating chain absorbing small}} &= \left(2 \sum_{r=1}^{\infty} \left\{ (2r-1)^{-2} \exp \left[- \frac{\pi^2 (2r-1)^2}{4\beta_N d^2} \right] \right. \right. \\
&\cdot \sin^2 \left[\frac{(2r-1)\pi\xi}{d} \right] + \left(\frac{16\beta_N d^2}{\pi^2} \right) \\
&\cdot \sum_{\substack{m, \ell=1 \\ m \neq \ell}}^{\infty} \left\{ [(2m-1)(2\ell-1)]^{-1} [(2m-1)^2 \right. \\
&- (2\ell-1)^2]^{-1} \cdot \exp \left[- \frac{\pi^2 (2\ell-1)^2}{4\beta_N d^2} \right] \\
&\cdot \left. \left. \sin \left[\frac{(2m-1)\pi\xi}{d} \right] \sin \left[\frac{(2\ell-1)\pi\xi}{d} \right] \right\} \right) \\
&\cdot \left\{ \sum_{p=1}^{\infty} (2p-1)^{-2} \exp \left[- \frac{\pi^2 (2p-1)^2}{4\beta_N d^2} \right] \right\}^{-1}
\end{aligned} \tag{53}$$

$$\begin{aligned}
\rho_{\text{cilium}}^{\text{absorbing small}} &= \left[\left(\frac{2}{d} \right) \sum_{r=1}^{\infty} \left\{ \exp \left[- \frac{\pi^2 (2r-1)^2}{4\beta_N d^2} \right] \right. \right. \\
&\quad \cdot \sin^2 \left[\frac{(2r-1)\pi\xi}{d} \right] + \left(\frac{8\beta_N d}{\pi^2} \right) \\
&\quad \left(\sum_{n=1}^{\infty} (2n-1)^{-1} \cdot \exp \left[- \frac{\pi^2 (2n-1)^2}{4\beta_N d^2} \right] \right. \\
&\quad \cdot \sin \left[\frac{(2n-1)\pi\xi}{d} \right] \cdot \left\{ \left(\frac{\pi}{2} \right) \left[1 - \left(\frac{\xi}{d} \right) \right] \right. \\
&\quad \left. \left. - [4(2n-1)]^{-1} \sin \left[\frac{(2n-1)\pi\xi}{d} \right] \right\} \right) \\
&\quad - \left(\frac{8\beta_N d}{\pi^2} \right) \sum_{\substack{\ell, m=1 \\ m \neq (2\ell-1)}}^{\infty} \{ [(2\ell-1)m^2 - (2\ell-1)^3]^{-1} \\
&\quad \cdot m \sin \left(\frac{m\pi\xi}{d} \right) \cdot \sin \left[\frac{(2\ell-1)\pi\xi}{d} \right] \\
&\quad \cdot \exp \left(- \frac{\pi^2 m^2}{4\beta_N d^2} \right) \} \cdot \left\{ \sum_{p=1}^{\infty} \exp \left[- \frac{\pi^2 (2p-1)^2}{4\beta_N d^2} \right] \right\}^{-1} \\
&\quad \left. \right] \quad (54)
\end{aligned}$$

$$\begin{aligned}
\rho_{\text{bridge}}^{\text{absorbing small}} &= \left(\frac{2}{d} \right) \left(\sum_{r=1}^{\infty} [r^2 (-1)^{r+1} \sin^2 \left(\frac{r\pi\xi}{d} \right) \right. \\
&\quad \cdot \exp \left(- \frac{\pi^2 r^2}{4\beta_N d^2} \right) \left. \right] + \left(\frac{8\beta_N d}{\pi^2} \right) \\
&\quad \cdot \sum_{n=1}^{\infty} \left((-1)^{n+1} n \sin \left(\frac{n\pi\xi}{d} \right) \exp \left(- \frac{\pi^2 n^2}{4\beta_N d^2} \right) \right)
\end{aligned}$$

$$\begin{aligned}
& \cdot \left\{ \left(\frac{\pi}{2} \right) \left[1 - \left(\frac{\xi}{d} \right) \right] \cos \left(\frac{n\pi\xi}{d} \right) - (4n)^{-1} \right. \\
& \cdot \left. \sin \left(\frac{n\pi\xi}{d} \right) \right\} - \left(\frac{8\beta_N d}{\pi^2} \right) \\
& \cdot \sum_{\substack{\ell, m=1 \\ \ell \neq m}}^{\infty} [(m^2 - \ell^2)^{-1} (-1)^{\ell+1} \ell m \sin \left(\frac{\ell\pi\xi}{d} \right) \\
& \cdot \sin \left(\frac{m\pi\xi}{d} \right) \exp \left(- \frac{\pi^2 m^2}{4\beta_N d^2} \right)] \\
& \cdot \left\{ \sum_{p=1}^{\infty} (-1)^{p+1} p^2 \exp \left(- \frac{p^2 \pi^2}{4\beta_N d^2} \right) \right\}^{-1} \quad (55)
\end{aligned}$$

$$\begin{aligned}
\rho_{\text{loop}} & \text{absorbing large} \\
& = (8\beta_N) \left[\xi \exp(-4\beta_N \xi^2) + 2 \sum_{n=1}^{\infty} \{ (nd + \xi) \right. \\
& \cdot \exp[-4\beta_N (nd + \xi)^2] - (nd) \exp(-4\beta_N n^2 d^2) \} \\
& + \sum_{\ell, m=1}^{\infty} \left([(\ell + m)d + \xi] \{ \exp -4\beta_N [(\ell + m)d \right. \\
& + \xi]^2 \} - 2 [(\ell + m)d] \{ \exp -4\beta_N [(\ell + m)d]^2 \} \\
& + [(\ell + m)d - \xi] \exp\{-4\beta_N [(\ell + m)d - \xi]^2\} \} \Big] \\
& \cdot \left\{ 1 + 2 \sum_{p=1}^{\infty} [1 - 8\beta_N (pd)^2] \exp[-4\beta_N (dp)^2] \right\}^{-1} \\
& \quad (56)
\end{aligned}$$

$$\begin{aligned}
\rho_{\text{floating chain}} &= \left[1 - 2(1 + 2\beta_N \xi^2) \operatorname{erfc}(\beta_N^{\frac{1}{2}} \xi) \right. \\
&\quad + (4\xi) \left(\frac{\beta_N}{\pi}\right)^{\frac{1}{2}} \exp(-\beta_N \xi^2) + (1 + 8\beta_N \xi^2) \\
&\quad \cdot \operatorname{erfc}(2\beta_N^{\frac{1}{2}} \xi) - (4\xi) \left(\frac{\beta_N}{\pi}\right)^{\frac{1}{2}} \exp(-4\beta_N \xi^2) \\
&\quad + 2 \sum_{n=1}^{\infty} (-1)^n \{ [1 + 2\beta_N (nd + 2\xi)^2] \\
&\quad \cdot \operatorname{erfc}[\beta_N^{\frac{1}{2}} (nd + 2\xi)] - \left(\frac{4\beta_N}{\pi}\right)^{\frac{1}{2}} \\
&\quad \cdot (nd + 2\xi) \exp[-\beta_N (nd + 2\xi)^2] \\
&\quad - [1 + 2\beta_N (nd + \xi)^2] \operatorname{erfc}[\beta_N^{\frac{1}{2}} (nd + \xi)] \\
&\quad + \left(\frac{4\beta_N}{\pi}\right)^{\frac{1}{2}} (nd + \xi) \exp[-\beta_N (nd + \xi)^2] \\
&\quad - (1 + 2\beta_N n^2 d^2) \operatorname{erfc}(\beta_N^{\frac{1}{2}} nd) \\
&\quad + \left(\frac{4\beta_N}{\pi}\right)^{\frac{1}{2}} (nd) \exp(-\beta_N n^2 d^2) \\
&\quad + [1 + 2\beta_N (nd - \xi)^2] \operatorname{erfc}[\beta_N^{\frac{1}{2}} (nd - \xi)] \\
&\quad - \left(\frac{4\beta_N}{\pi}\right)^{\frac{1}{2}} (nd - \xi) \exp[-\beta_N (nd - \xi)^2] \} \\
&\quad + \sum_{\ell, m=1}^{\infty} (-1)^{\ell+m} \left(\{1 + 2\beta_N [(\ell + m)d \right. \\
&\quad \left. + 2\xi]^2 \} \operatorname{erfc}[\beta_N^{\frac{1}{2}} [(\ell + m)d + 2\xi]] \right.
\end{aligned}$$

$$\begin{aligned}
& - \left(\frac{4\beta_N}{\pi}\right)^{\frac{1}{2}} [(\ell + m)d + 2\xi] \\
& \cdot \exp\{-\beta_N [(\ell + m)d + 2\xi]^2\} \\
& - 2\{1 + 2\beta_N [(\ell + m)d]^2\} \\
& \cdot \operatorname{erfc}\{\beta_N^{\frac{1}{2}} [(\ell + m)d]\} + 2\left(\frac{4\beta_N}{\pi}\right)^{\frac{1}{2}} \\
& \cdot [(\ell + m)d] \exp\{-\beta_N [(\ell + m)d]^2\} \\
& + \{1 + 2\beta_N [(\ell + m)d - 2\xi]^2\} \\
& \cdot \operatorname{erfc}\{\beta_N^{\frac{1}{2}} [(\ell + m)d - 2\xi]\} \\
& - \left(\frac{4\beta_N}{\pi}\right)^{\frac{1}{2}} [(\ell + m)d - 2\xi] \\
& \cdot \exp\{-\beta_N [(\ell + m)d - 2\xi]^2\} \Bigg] \\
& \cdot \left(1 + \{4\sum_{p=1}^{\infty} (-1)^p p \operatorname{erfc}[\beta_N (pd)^2]\}\right. \\
& - 2(\beta_N \pi d^2)^{-\frac{1}{2}} - 4(\beta_N \pi d^2)^{-\frac{1}{2}} \\
& \cdot \left.\left\{\sum_{s=1}^{\infty} (-1)^s \exp[-\beta_N (sd)^2]\right\}\right)^{-1}
\end{aligned}$$

(57)

$$\begin{aligned}
\rho_{\text{cilium}}^{\text{absorbing large}} &= (4\pi\beta_N)^{\frac{1}{2}} \left[\operatorname{erfc}(\beta_N^{\frac{1}{2}}\xi) - \operatorname{erfc}(2\beta_N^{\frac{1}{2}}\xi) \right. \\
&+ \sum_{n=1}^{\infty} \{ (-1)^n \operatorname{erfc}(\beta_N^{\frac{1}{2}}nd) - (-1)^n \\
&\cdot \operatorname{erfc}[\beta_N^{\frac{1}{2}}(nd + 2\xi)] + \operatorname{erfc}[\beta_N^{\frac{1}{2}}(2nd + \xi)] \\
&- \operatorname{erfc}[\beta_N^{\frac{1}{2}}(2nd + 2\xi)] + \operatorname{erfc}(\beta_N^{\frac{1}{2}}2nd) \\
&- \operatorname{erfc}[\beta_N^{\frac{1}{2}}(2nd - \xi)] \} + \sum_{\ell, m=1}^{\infty} (-1)^{\ell} \\
&\cdot \left(2\operatorname{erfc}[\beta_N^{\frac{1}{2}}(\ell + 2m)d] - \operatorname{erfc}[\beta_N^{\frac{1}{2}}[(\ell + 2m)d \right. \\
&+ 2\xi]] - \operatorname{erfc}[\beta_N^{\frac{1}{2}}[(\ell + 2m)d - 2\xi]] \Big) \\
&\cdot \{ 1 + 2 \sum_{p=1}^{\infty} (-1)^p \exp[-\beta_N (pd)^2] \}^{-1} \quad (58)
\end{aligned}$$

$$\begin{aligned}
\rho_{\text{bridge}}^{\text{absorbing large}} &= (\beta_N) \left[\sum_{n=1}^{\infty} \left([(2n - 1)d] \exp\{-\beta_N [(2n - 1)d]^2\} \right. \right. \\
&- [(2n - 1)d + 2\xi] \exp\{-\beta_N [(2n - 1)d + 2\xi]^2\} \\
&- \sum_{\ell, m=1}^{\infty} [(2m + 2\ell - 1)d + 2\xi] \\
&\cdot \exp\{-\beta_N [(2m + 2\ell - 1)d + 2\xi]^2\} \\
&- 2[(2m + 2\ell - 1)d] \exp\{-\beta_N [(2m + 2\ell - 1)d]^2\} \\
&+ [(2m + 2\ell - 1)d - 2\xi] \exp\{-\beta_N [(2m + 2\ell - 1)d
\end{aligned}$$

$$\begin{aligned}
& - 2\xi]^2\} \Bigg] \cdot \left(\sum_{p=1}^{\infty} [2\beta_N (2p-1)^2 d^2 - 1] \right. \\
& \left. \cdot \exp\{-\beta_N [(2p-1)d]^2\} \right)^{-1} \quad (59)
\end{aligned}$$

$$\begin{aligned}
\rho_{\text{loop reflecting small}} &= \left[\left(\frac{1}{d} \right) + \left(\frac{4\beta_N \xi^2}{d^2} \right) - \left(\frac{8\beta_N \xi}{d} \right) + \left(\frac{8\beta_N}{3} \right) + \left(\frac{4}{d^2} \right) \right. \\
&\quad \cdot \sum_{r=1}^{\infty} \left[\cos^2 \left(\frac{r\pi\xi}{d} \right) \cdot \exp\left(-\frac{\pi^2 r^2}{4\beta_N d^2}\right) \right] + \left(\frac{16\beta_N}{\pi^2} \right) \\
&\quad + \sum_{n=1}^{\infty} \left(\cos \left(\frac{n\pi\xi}{d} \right) \exp\left(-\frac{\pi^2 n^2}{4\beta_N d^2}\right) \right. \\
&\quad \cdot \{ (2n^2)^{-1} \cos \left(\frac{n\pi\xi}{d} \right) + (2n)^{-1} (\pi) \\
&\quad \cdot \left[\left(\frac{\xi}{d} \right) - 1 \right] \sin \left(\frac{n\pi\xi}{d} \right) \} \Bigg] \\
&\quad \cdot \left[\left(\frac{1}{d} \right) + \left(\frac{2}{d} \right) \sum_{p=1}^{\infty} \exp\left(-\frac{\pi^2 p^2}{4\beta_N d^2}\right) \right]^{-1} \quad (60)
\end{aligned}$$

$$\rho_{\text{floating chain reflecting small}} = 1 \quad (61)$$

$$\begin{aligned}
\rho_{\text{cilium reflecting small}} &= \left(\frac{1}{d} \right) + \left(\frac{2\beta_N \xi^2}{d} \right) + \left(\frac{4\beta_N d}{3} \right) - (4\beta_N \xi) - \left(\frac{8\beta_N d}{\pi^2} \right) \\
&\quad \cdot \sum_{r=1}^{\infty} \left[(r)^{-2} \exp\left(-\frac{\pi^2 r^2}{4\beta_N d^2}\right) \cdot \cos \left(\frac{r\pi\xi}{d} \right) \right] \quad (62)
\end{aligned}$$

$$\begin{aligned}
\rho_{\text{bridge reflecting small}} &= \left[\left(\frac{1}{d^2} \right) + \left(\frac{4\beta_N \xi^2}{d^2} \right) - \left(\frac{4\beta_N \xi}{d} \right) + \left(\frac{2\beta_N}{3} \right) - \left(\frac{8\beta_N}{\pi^2} \right) \right. \\
&\quad \cdot \sum_{r=1}^{\infty} \{ [1 + (-1)^r] \cdot (r)^{-2} \cos \left(\frac{r\pi \xi}{d} \right) \\
&\quad \cdot \exp \left(- \frac{r^2 \pi^2}{4\beta_N d^2} \right) + \left(\frac{4}{d^2} \right) \sum_{n=1}^{\infty} \{ (-1)^n \\
&\quad \cdot \cos^2 \left(\frac{n\pi \xi}{d} \right) \exp \left(- \frac{n^2 \pi^2}{4\beta_N d^2} \right) + \left(\frac{16\beta_N}{\pi^2} \right) \\
&\quad \cdot \sum_{s=1}^{\infty} \left((-1)^s \cos \left(\frac{s\pi \xi}{d} \right) \exp \left(- \frac{\pi^2 s^2}{4\beta_N d^2} \right) \right. \\
&\quad \cdot \{ (2s^2)^{-1} + (4s^2)^{-1} \cos \left(\frac{s\pi \xi}{d} \right) + \left(\frac{\pi}{2s} \right) \\
&\quad \left. \left[\left(\frac{\xi}{d} \right) - 1 \right] \sin \left(\frac{s\pi \xi}{d} \right) \} \right) - \left(\frac{16\beta_N}{\pi^2} \right) \\
&\quad \cdot \sum_{\substack{\ell, m=1 \\ \ell \neq m}}^{\infty} [(-1)^m (\ell^2 - m^2)^{-1} \cos \left(\frac{\ell \pi \xi}{d} \right) \\
&\quad \cdot \cos \left(\frac{m \pi \xi}{d} \right) \exp \left(- \frac{\pi^2 \ell^2}{4\beta_N d^2} \right)] \cdot \left\{ \left(\frac{1}{d} \right) \right. \\
&\quad \left. + \left(\frac{2}{d} \right) \left[\sum_{p=1}^{\infty} (-1)^p \exp \left(- \frac{p^2 \pi^2}{4\beta_N d^2} \right) \right] \right\}^{-1} \quad (63)
\end{aligned}$$

$$\begin{aligned}
\rho_{\text{loop reflecting large}} &= (4\beta_N \pi)^{\frac{1}{2}} \left[\operatorname{erfc}(2\beta_N^{\frac{1}{2}} \xi) + 2 \sum_{r=1}^{\infty} \operatorname{erfc}(2\beta_N^{\frac{1}{2}} r d) \right. \\
&\quad + \left. \operatorname{erfc}[2\beta_N^{\frac{1}{2}} (r d + \xi)] \right] + \sum_{\ell, m=1}^{\infty} \left(\operatorname{erfc}[2\beta_N^{\frac{1}{2}} \right. \\
&\quad \cdot [(\ell + m)d + \xi]] + 2 \operatorname{erfc}[2\beta_N^{\frac{1}{2}} [(\ell + m)d]] \\
&\quad + \left. \operatorname{erfc}[2\beta_N^{\frac{1}{2}} [(\ell + m)d - \xi]] \right) \Bigg] \\
&\quad \cdot \left\{ 1 + 2 \sum_{p=1}^{\infty} \exp[-\beta_N (p d)^2] \right\}^{-1} \quad (64)
\end{aligned}$$

$$\rho_{\text{floating chain reflecting}} = 1 \quad (65)$$

$$\begin{aligned}
\rho_{\text{cilium reflecting large}} &= \left(\frac{16\beta_N}{\pi} \right)^{\frac{1}{2}} \left(\exp(-\beta_N \xi^2) - (\beta_N \pi)^{\frac{1}{2}} \xi \right. \\
&\quad \cdot \operatorname{erfc}(\beta_N^{\frac{1}{2}} \xi) + \sum_{r=1}^{\infty} \exp[-\beta_N (2rd - \xi)^2] \\
&\quad + \left. \exp[-\beta_N (2rd + \xi)^2] \right\} - (\beta_N \pi)^{\frac{1}{2}} \\
&\quad \cdot \sum_{n=1}^{\infty} \{ (2nd - \xi) \operatorname{erfc}[\beta_N^{\frac{1}{2}} (2nd - \xi)] \\
&\quad + (2nd + \xi) \operatorname{erfc}[\beta_N^{\frac{1}{2}} (2nd + \xi)] \} \quad (66)
\end{aligned}$$

$$\begin{aligned}
\rho_{\text{bridge}} &= (\beta_N \pi)^{\frac{1}{2}} \left[\sum_{r=1}^{\infty} \left(\operatorname{erfc}\{\beta_N^{\frac{1}{2}}[(2r-1)d + 2\xi]\} \right. \right. \\
&\quad \left. \left. + \operatorname{erfc}\{\beta_N^{\frac{1}{2}}[(2r-1)d]\} \right) \right. \\
&\quad + \sum_{\ell, m=1}^{\infty} \left(\operatorname{erfc}\{\beta_N^{\frac{1}{2}}[(2m+2\ell-1)d + 2\xi]\} \right. \\
&\quad + 2\operatorname{erfc}\{\beta_N^{\frac{1}{2}}[(2m+2\ell-1)d]\} \\
&\quad \left. \left. + \operatorname{erfc}\{\beta_N^{\frac{1}{2}}[(2m+2\ell-1)d - 2\xi]\} \right) \right] \\
&\quad \cdot \left\{ \sum_{p=1}^{\infty} \exp[-\beta_N(2p-1)^2 d^2] \right\}^{-1} \quad (67)
\end{aligned}$$

Equations (52) through (67) are not normalized. The normalization condition is $\int_0^d \rho d\xi = 1$.

5. DISCUSSION

The segment density profiles of the various types of confined chains are shown qualitatively in Figures 1 through 4. When the walls are reflecting, the segment density of a cilium, bridge or loop is greatest at the wall or walls to which it is attached. The segment density of the cilium or loop decreases monotonically with increasing distance from the wall of attachment while the segment density profile of the bridge is symmetric about its minimum which occurs midway between the walls. The floating chain is the only chain which has a constant segment density profile. When the walls are absorbing, the segment densities of all of the chains are zero at the walls and pass through a maximum. The maximum for the loop or cilium occurs at a distance less than halfway from the wall of attachment to the opposing wall. The maximum in the segment density of the bridge or floating chain occurs midway between the walls and the profile is symmetric about this position.

Figure 1. The segment density profile of a loop confined between two infinite parallel walls separated by a distance d .
(- - - -) reflecting walls; (——) absorbing walls.

Figure 2. The segment density profile of a cilium. (- - - -) reflecting walls; (——) absorbing walls.

Figure 3. The segment density profile of a floating chain. (- - - -) reflecting walls; (————) absorbing walls.

Figure 4. The segment density profile of a bridge. (- - - -) reflecting walls; (————) absorbing walls.

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APPENDIX

Figure 5. Flowchart of the main computer program designed to generate the previous curves.

Figure 6. Flowchart of a subprogram used by the main computer program to evaluate infinite series.

```

1      PROGRAM SEGDEMS (INPUT,OUTPUT)
      REAL A,B,C,D,X(100),Y(100),PI,G,H
      INTEGER I
      PI=3.14159
5      B=0.0001
      D=100.
      C=PI*PI/4/R/D/D*(-1)
      G=SQRT(B)
      H=2*G/(SQRT(PI))
10     C      PLOT THE RESULTS FOR LOOP (ABS,SMALL)
      DO 10 I=1,100
          A=PI*I/D
          F=PI/2*(1-I/D)
          Y(I)=(2/D*SUM(2,A,2,0,0,C,1,0,0,0,0,0,1,1)+16*B*D/PI/PI*SUM
15     * (1,A,1,0,0,C,F,0,A,.25,1,A,1,1))/SUM(2,A,0,0,0,C,1,0,0,0,0,0,1,1)
          X(I)=I
10     CONTINUE
      CALL GRAPH(X,Y,100,"E","PLCCP(AES","SMALL)")
      C      PLOT THE RESULTS FOR CILIUM (ABS,SMALL)
20     DO 20 I=1,100
          A=PI*I/D
          F=PI/2*(1-I/D)
          Y(I)=(2/D*SUM(0,A,2,0,0,C,1,0,0,0,0,0,1,2)+8*B*D/PI/PI*
25     * SUM(-1,A,1,0,0,C,F,0,A,.25,1,A,1,2)-8*B*D/PI/PI*SSUM(1,0,2,1,0,3
      * ,0,0,A,1,C,1,1,0))/SUM(C,A,C,0,0,C,1,0,0,0,0,0,1,2)
          X(I)=I
20     CONTINUE

```

```

30      CALL GRAPH(X,Y,100,"E","PCILIUM(AB","S,SMALL)")
C      PLOT THE RESULT FOR FLOATING CHAIN(ABS,SMALL)
      DO 30 I=1,100
        A=PI*I/D
        F=PI/2*(1-I/D)
        Y(I)=1/2*SUM(-2,A,2,0,0,C,1,0,0,0,0,0,1,2)+16*B*D*PI/PI*
*      SSUM(0,0,3,2,2,3,0,0,A,A,1,C,1,1,1)/SUM(-2,A,0,0,0,C,1,0,0,0,0
*      X(I)=I
      CONTINUE
30      CALL GRAPH(X,Y,100,"E","P FC (ABS","SMALL)")
C      PLOT THE RESULT FOR THE BRIDGE(ABS,SMALL)
      DO 40 I=1,100
        A=PI*I/D
        F=PI/2*(1-I/D)
        Y(I)=2/D*(SUM(2,A,2,0,0,C,-1,0,0,0,0,0,-1,1)-8*B*D/PI/PI*
*      SUM(1,A,1,0,0,C,-F,0,A,-2,1,A,-1,1)-8*B*D/PI/PI*SSUM(1,1,0,2,2
*      ,0,0,0,-A,A,1,C,-1,-1,-1)/SUM(2,A,0,0,0,C,-1,0,0,0,0,0,-1,1)
        X(I)=I
      CONTINUE
40      CALL GRAPH(X,Y,100,"E","PBRIDGE(AB","S,SMALL)")
C      PLOT THE RESULTS FOR THE LOOP(REFL,SMALL)
      DO 50 I=1,100
        A=PI*I/D
        F=PI/2*(1-I/D)
        Y(I)=1/D/D+4*B*I*I/D/D-8*B*I/D+8*B/3+4/D/D*SUM(0,A,0,A,2,C,1
*      ,0,0,0,0,0,1,1)+16*B/PI/PI*SUM(-1,A,0,A,1,C,.5,1,A,-F,0,A,1,1)
*      )*(1/D+2/D*SUM(0,A,0,0,0,C,1,0,0,0,0,0,1,1))
        X(I)=I
      CONTINUE
50

```

```

60      CALL GRAPH(X,Y,100,"E","PLOOP(REFL","SMALL)")
C      PLOT FOR THE CILIUM(REFL,SMALL)
DO 60 I=1,100
      A=PI*I/D
      F=PI/2*(1-I/D)
      Y(I)=1/D+2*B*I*I/D+4*B*D/3-4*B*I-8*B*D/PI/PI*
*      SUM(-2,A,0,0,0,C,1.,0,0,0,0,0,1,1)
65      X(I)=I
      CONTINUE
60      CALL GRAPH(X,Y,100,"E","PCILIUM(RE","FL,SMALL)")
C      PLOT THE RESULT FOR THE BRIDGE(REFL,SMALL)
DO 70 I=1,100
      F=PI/2*(1-I/D)
      A=PI*I/D
      Y(I)=(1/D/D+4*B*I*I/D/D-4*B*I/D+2*B/3-8*B/PI/PI*BSUM(1,2,A,C,
*      0,0,A,0)+4/D/D*SUM(0,A,C,A,2,C,1.,0,0,0,0,0,-1,1)
*      +16*B/PI/PI*BSUM(0,1,A,C,A,F,A,1)
75      *M(0,0,2,0,0,2,A,A,A,A,0,C,-1,-1,-1))/(2/D*SUM(0,A,0,0,0,C,1.,0,0,0
*      0,0,-1,1)*(-1))
      X(I)=I
70      CONTINUE
      CALL GRAPH(X,Y,100,"E","PBRIDGE(RE","FL,SMALL)")
80      C      PLOT THE RESULTS FOR THE LOOP(AES,LARGE)
DO 80 I=1,100
      Y(I)=8*B*(I*EXP(-4*B*I*I)+2*EXSUM(4,1,I,0,1,0,1,0,1,0)
*      -2*EXSUM(4,1,0,0,1,0,1,1,0)+EXSUM(4,1,-1,0,4,0,1,1,0)
*      -2*EXSUM(4,1,0,0,4,0,1,1,0)+EXSUM(4,1,-1,0,4,0,1,1,0))
85      *      /(1+2*EXSUM(4,1,0,1,1,1,-8,1,0))
      X(I)=I
80      CONTINUE
      CALL GRAPH(X,Y,100,"E","PLOOP(AES","LARGE)")
C      PLOT THE RESULTS FOR THE CILIUM(AES,LARGE)

```

```

90      DO 85 I=1,100
      Y(I)=SQRT(4*PI*B)*(ERFC(G*I)-ERFC(2*G*I)+ERSUM(1,0,0,-1,1,0,1
*      ,1)-ERSUM(1,2*I,0,-1,1,0,1,1)+ERSUM(2,1,0,1,1,0,1,1)
*      -ERSUM(2,2*I,0,1,1,1,0,1)+ERSUM(2,0,0,1,1,1,0,1)
*      -ERSUM(2,-1,0,1,1,1,0,1)+ERSUM(1,0,0,-1,1,0,1,3)*2
95      -ERSUM(1,2*I,0,-1,1,0,1,3)-ERSUM(1,-2*I,0,-1,1,0,1,3)
*      )/(-(1+2*EXSUM(1,1,0,0,1,0,1,-1,0)))
      X(I)=I
85      CONTINUE
      CALL GRAPH(X,Y,100,"E","PCILIUM(AB)","S,LARGE")
100     C      PLOT THE RESULTS FOR THE FLOATING CHAIN(AES,LARGE)
      DO 90 I=1,100
      Y(I)=(1-2*(1+2*B*I*I)*ERFC(G*I)+H*I*EXP(-B*I*I)*2
*      + (1+8*B*I*I)*ERFC(2*G*I)-H*I*EXP(-4*B*I*I)*2
*      +2*(ERSUM(1,2*I,1,-1,1,1,1,1)-EXSUM(1,1,2*I,0,1,0,1,-1,0)*H
*      -ERSUM(1,1,1,-1,1,1,1,1)+EXSUM(1,1,1,0,1,0,1,-1,0)*H
*      -ERSUM(1,0,1,-1,1,1,1,1)+EXSUM(1,1,0,0,1,0,1,-1,0)*H
*      +ERSUM(1,-1,1,-1,1,1,1,1)-EXSUM(1,1,-1,0,1,0,1,-1,0)*H)
*      +ERSUM(1,2*I,1,-1,1,1,1,4)-EXSUM(1,1,2*I,0,4,0,1,-1,0)*H
*      -(ERSUM(1,0,1,-1,1,1,1,4)-EXSUM(1,1,0,0,4,0,1,-1,0)*H)*2
110     +ERSUM(1,-2*I,1,-1,1,1,1,4)-EXSUM(1,1,-2*I,0,4,0,1,-1,0)*H
*      )/(1+4*ERSUM(1,0,0,-1,1,0,1,1)-2/SQRT(B*PI*D*D)-4/SQRT
*      (B*PI*D*D)*EXSUM(1,1,0,0,1,0,1,-1,0))
      X(I)=I
90      CONTINUE

```

115

C CALL GRAPH(X,Y,100,"E","P FC (AES","LARGE) ")
 PLOT THE RESULTS FOR THE BRIDGE (ABS,LARGE)
 DO 92 I=1,100

120

* Y(I)=B*(EXSUM(1,1,0,0,2,0,1,1,0)-EXSUM(1,1,2*I,0,2,0,1,1,0)
 * -EXSUM(1,1,2*I,0,5,0,1,1,0)+2*EXSUM(1,1,0,0,5,0,1,1,0)
 * -EXSUM(1,1,-2*I,0,5,0,1,1,0))/EXSUM(1,1,0,1,2,1,2,2,2)

92

CONTINUE
 C CALL GRAPH(X,Y,100,"E","P BRIDGE (AB","S,LARGE) ")
 PLOT THE RESULTS FOR THE LOOP (REFL,LARGE)
 DO 94 I=1,100

125

* Y(I)=SQRT(4*B*PI)*(ERFC(2*G*I)+2*ERSUM(1,0,0,1,2,1,1,1)
 * +2*ERSUM(1,1,0,1,2,1,1,1)+ERSUM(1,1,0,1,2,1,1,4)
 * +2*ERSUM(1,0,0,1,2,1,1,4)+ERSUM(1,-1,0,1,2,1,1,4))
 * /((1+EXSUM(1,1,0,0,1,1,0,0,1,0))

130

94

CONTINUE
 C CALL GRAPH(X,Y,100,"E","P LOOP (REF","L,LARGE) ")
 PLOT THE RESULTS FOR THE CILIUM (REFL,LARGE)
 DO 96 I=1,100

135

* Y(I)=H*(EXP(-B*I*I)-SQRT(B*PI)*I*ERFC(G*I)+EXSUM(1,2,-I,0,1,
 * 1,0,1,0)+EXSUM(1,2,I,0,1,1,0,1,0)-SQRT(B*PI)*(ERSUM
 * (2,-I,-2,1,1,0,0,1)+ERSUM(2,I,-2,1,1,0,0,1))*4)*8

140

96

CONTINUE
 C CALL GRAPH(X,Y,100,"E","P CILIUM (E","FL,LARGE) ")
 PLOT THE RESULTS FOR THE BRIDGE (EFFL,LARGE)
 DO 98 I=1,100

145

* Y(I)=SQRT(B*PI)*(ERSUM(1,2*I,0,1,1,1,1,2)+ERSUM(1,0,0,1,1,1,1,
 * 1,2)+ERSUM(1,2*I,0,1,1,1,1,5)+ERSUM(1,0,0,1,1,1,1,5))*2,
 * +ERSUM(1,-2*I,0,1,1,1,1,5))/EXSUM(1,1,0,0,2,1,0,1,0)

98

CONTINUE
 C CALL GRAPH(X,Y,100,"E","P BRIDGE (LE","FL,LARGE) ")
 STOP
 END

150

```

1      REAL FUNCTION SUM(S1,S2,S3,S4,S5,S6,S7,S8,S9,S10,S11,S12,S13,S14)
C      SINGLE SUMMATION ALGORITHMS
      INTEGER S1,S3,S5,S8,S11,S13,S14
      REAL S2,S4,S6,S7,S9,S10,S12
5      INTEGER M,J,K
      REAL A(20),PARTS,RATIO
      J=0
      K=0
      PARTS=0
10     CONTINUE
C     THE NATURE OF THE COUNTING OF THE SERIES WILL BE DETERMINED.
      IF (S14.EQ.1) M=J+1
      IF (S14.EQ.2) M=2*J+1
      IF (K.EQ.3) GO TO 40
15     C     THE GENERAL EQUATION OF THE SMALL WALL FORM IS REPRESENTED NOW
      A(M)=1**S1*(SIN(S2*M))**S3*(COS(S4*M))**S5*EXP(S6*M*M)*
      * (S7*COS(S9*M)/M**S8-S10*SIN(S12*M)/M**S11)*(S13)**M
      PARTS=PARTS+A(M)
      RATIO=A(M)/PARTS
20     IF (.NOT.(RATIO.LT.0.0001)) GO TO 20
      K=3
      SUM=PARTS
20     CONTINUE
      IF (M.NE.20) GO TO 30
25     SUM=10.**10.
30     CONTINUE
      J=J+1
      GO TO 10
40     CONTINUE
30     RETURN
      END

```

```

1      REAL FUNCTION SSUM(S1,S2,S3,S4,S5,S6,S7,S8,S9,S10,S11,S12,S13,S14,
*      S15)
C      DOUBLE SUMMATION ALGORITHMS
5      INTEGER S1,S2,S3,S4,S5,S6,S11,S13,S14,S15
      REAL S7,S8,S9,S10,S12
      INTEGER I,J,K,L,M,N
      REAL PARTS,A(20,20),RATIO
      K=0
      PARTS=0
10     L=1
      N=0
      CONTINUE
      IF (S14) 20,30,40
20     I=K+1
      GO TO 50
30     J=K+1
      GO TO 50
40     J=2*K+1
50     CONTINUE
      IF (N.EQ.3) GO TO 25
      DO 15 M=1,2
60         IF (S15) 60,70,80
            J=L+1
            GO TO 90
70         J=2*L+1
            GO TO 90
80         J=2*L+1
90         CONTINUE
      C      THE GENERAL FORM OF THE SMALL WALL FORM IN THE CASE OF THE DOUBLE
      C      SERIES IS REPRESENTED
30     A(I,J)=1.*J**S1*I**S2/(I**S3*J**S4-I**S5*J**S6)*COS(I*S7)
*      *COS(J*S8)*(SIN(I*S9)*SIN(J*S10))**S11*EXP(S12*I*I)*(S13)**J
      PARTS=PARTS+A(I,J)
      RATIO=A(I,J)/PARTS
      L=L+1
35     IF (RATIO.GE.0.001) GO TO 5
      N=N+1
      SSUM=PARTS
      CONTINUE
40     CONTINUE
      K=K+1
      GO TO 10
25     CONTINUE
45     RETURN
      END

```

```

1      REAL FUNCTION BSUM(S1,S2,S3,S4,S5,S6,S7,S8)
      INTEGER S1,S2,S8
      REAL S3,S4,S5,S6,S7
      INTEGER M,J,K
5      REAL A(20),PARTS,RATIO
      J=0
      K=0
      PARTS=0
10     CONTINUE
      M=J+1
      IF (K.EQ.3) GO TO 40
      A(M)=FLOAT(S1+(-1)**M)/FLOAT(M**S2)*COS(S3*M)*EXP(S4*M*M)
      * (.5/M+.25/M**2)*COS(S5*M)-S6*SIN(S7*M)**S8
      PARTS=PARTS+A(M)
15     IF (PARTS.EQ.0) GO TO 20
      RATIO=A(M)/PARTS
      IF (.NOT.(RATIO.LT.0.0001)) GO TO 20
      K=3
      BSUM=PARTS
20     CONTINUE
      IF (M.NE.20) GO TO 30
      BSUM=10.**10
30     CONTINUE
      J=J+1
      GO TO 10
25     CONTINUE
40     RETURN
      END

```



```

1      REAL FUNCTION ERFC (X)
      REAL X
      REAL A1,A2,A3,A4
      A1=0.27839
5      A2=0.23039
      A3=0.000972
      A4=0.078108
      ERFC= ((( (A4*X+A3)*X) + A2)*X+A1)*X+1) ** (-4)
10     RETURN
      END

```

```

1      REAL FUNCTION ERSUM (S1,S2,S3,S4,S5,S6,S7,S8)
      INTEGER S1,S2,S3,S4,S5,S6,S7,S8
      INTEGER I,J,K
      REAL PARTS,A(20),RATIO,B,D
5      J=0
      K=0
      PARTS=0
      D=100.
      B=0.0001
10     CONTINUE
      IF (S8.EQ.1)      I=J+1
      IF (S8.EQ.2)      I=2*J+1
      IF (S8.EQ.3)      I=J+3
      IF (S8.EQ.4)      I=J+2
15     IF (S8.EQ.5)      I=2*J+3
      IF (K.EQ.3)      GO TO 30
      A(I)=(S7+2*B**S6*(S1*I*D+S2)**2)**S3*ERFC(S5*SQRT(B)*(S1*I*D
*      +S2))* (S4)**I
      PARTS=PARTS+A(I)
      RATIO=A(I)/PARTS
20     IF (.NOT. (ABS(RATIO).LT.0.001)) GO TO 20
      K=3
      ERSUM=PARTS
      CONTINUE
25     J=J+1
      GO TO 10
30     CONTINUE
      RETURN
      END

```

```

1      REAL FUNCTION EXSUM(S1,S2,S3,S4,S5,S6,S7,S8,S9)
      INTEGER S1,S2,S3,S4,S5,S6,S7,S8,S9
      INTEGER I,J,K
      REAL PARTS,A(20),RATIO,B,D
      J=0
      K=0
      PARTS=0
      D=100.
      P=C.0001
10      CONTINUE
      IF(S5.EQ.1)      I=J+1
      IF(S5.EQ.2)      I=2*J+1
      IF(S5.EQ.3)      I=J+3
      IF(S5.EQ.4)      I=J+2
15      IF(S5.EQ.5)      I=2*J+3
      IF(K.EQ.3)      GO TO 30
      A(I)=(S6+S7*B**S4*D**S9*(S2*I*D+S3))*EXP(-S1*B*(S2*I*D+S3)
      *      **2)*(S8)**I
      PARTS=PARTS+A(I)
20      IF(PARTS.EQ.0)      GO TO 20
      RATIO=A(I)/PARTS
      IF(.NOT.(ABS(RATIO).LT.0.001)) GO TO 20
      K=3
      EXSUM=PARTS
25      CONTINUE
      J=J+1
      GO TO 10
30      CONTINUE
      RETURN
      END
30

```

```

1      SUBROUTINE GRAPH (X,Y,N,XNAME,YNAME1,YNAME2)
      INTEGER N
      REAL X(N),Y(N)
      INTEGER XNAME,YNAME1,YNAME2,LINE (119)
5      REAL YMIN,YMAX,YRANGE
      INTEGER COLUMN,XAXIS,YPRINT,I
      C      FIND THE RANGE OF Y TO BE PLOTTED
      CALL MINMAX(Y,N,YMIN,YMAX)
      YRANGE=YMAX-YMIN
10     C      CLEAR LINE TO BLANKS
      DO 10 COLUMN=1,119
10        LINE(COLUMN)=" "
      CONTINUE
      C      PLACE XAXIS MARK IN LINE
15     XAXIS=118*(0-YMIN)/YRANGE+1.5
      IF (.NOT.(XAXIS.GE.1.AND.XAXIS.LE.119)) GO TO 15
      LINE(XAXIS)="I"
      CONTINUE
15     LABEL GRAPH
      C      PRINT20,YNAME1,YNAME2,XNAME
20     FORMAT(1H1,10HGRAPH OF ,A10,A10,7HVERSUS ,A2)
      C      PREPARE AND PRINT THE LINES OF THE GRAPH
      DO 35 I=1,N
25        YPRINT=118*(Y(I)-YMIN)/YRANGE+1.5
25        LINE(YPRINT)="*"
        PRINT 25,X(I),LINE,Y(I)
        FORMAT(" ",F4.0,119A1,F9.3)
        IF (.NOT.(YPRINT.EQ.XAXIS)) GO TO 30
        LINE(YPRINT)="I"
        GO TO 35
30        LINE(YPRINT)=" "
30     CONTINUE
35     RETURN
      END

```

```

1      SUBROUTINE MINMAX(NUMBER,N,MIN,MAX)
C      THIS SUBROUTINE FINDS THE SMALLEST AND LARGEST VALUES FOR THE
C      SEGMENT DENSITIES
5      INTEGER N
      REAL NUMBER(N),MIN,MAX
      INTEGER I
      MIN=NUMBER(1)
      MAX=NUMBER(1)
10     DO 10 I=2,N
          IF (.NOT.(NUMBER(I).LT.MIN)) GO TO 20
              MIN=NUMBER(I)
              CONTINUE
20     IF (.NOT.(NUMBER(I).GT.MAX)) GO TO 30
              MAX=NUMBER(I)
              CONTINUE
15     30 CONTINUE
10     RETURN
      END

```