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Screening in a collection of crumpled manifolds

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The continuum theory of a collection of self-avoiding D-dimensional manifolds with fixed connectivity embedded in d dimensions is considered. The self-avoiding interaction between multiple points of a manifold is shown to be screened in the presence of other manifolds. The screening length and the mean-square distance between two points of a manifold are derived to decrease with the manifold density ρ according to $\rho^{-(D+2)/2(d-D)}$ and $\rho^{-[4D-(2-D)d]/2(d-D)}$, respectively.

There is currently considerable interest[1–5] in understanding the behavior of random surfaces. Specifically, the static and dynamic properties of a self-avoiding (SA) "tethered" (or "fixed connectivity") surface have been explored using Monte Carlo simulations and analytical calculations at one-loop level.[3–5] In this paper I consider a collection of SA manifolds and demonstrate using a variational calculation that the bare excluded volume interaction is screened. The scaling results for the dependence of correlation length and the mean-square distance between two points on a manifold on the manifold density are derived in the "hydrodynamic limit."

Consider N self-avoiding manifolds each of dimension D and fixed connectivity, embedded in d-dimensional space. The internal space of αth manifold is described by a coordinate $x_\alpha=\{x_\alpha^1,\dots,x_\alpha^D\}$ in a bounded $\mathcal{V}$ of of $\mathbb{R}^D$. The position in d space is $\mathbf{r}_\alpha(x_\alpha)$. The probability distribution is given by the generalized Edwards model,[4–6]

$$\mathcal{P}(\{\mathbf{r}_\alpha\})=\exp\left[-\frac{1}{2a}\sum_{\alpha=1}^{N}\int d^Dx_\alpha[\nabla\mathbf{r}_\alpha(x_\alpha)]^2-\frac{w}{2}\sum_{\alpha,\beta=1}^{N}\int d^Dx_\alpha\int d^Dx_\beta\,\delta^D(\mathbf{r}_\alpha(x_\alpha)-\mathbf{r}_\beta(x_\beta))\right], \quad (1)$$

where

$$(\nabla\mathbf{r}_\alpha)^2=\sum_{i=1}^{D}(\partial\mathbf{r}_\alpha/\partial x_{\alpha i})^2$$

and a^{-1} correspond, respectively, to the Gaussian potential and the elastic coefficient of a free tethered manifold, while w measures the strength of the "excluded volume" interaction. As in the case of polymers, a is some coarse-grained bare "lattice volume." There is a cutoff volume λ in the self-excluded volume term corresponding to a minimum internal distance across which the manifold can self-interact.[7] I consider below the limit of $\lambda/\mathcal{V}\to 0$. For a single Gaussian tethered manifold ($w=0$),

$$\begin{aligned}\langle\exp\{i\mathbf{k}\cdot[\mathbf{r}(x_1)-\mathbf{r}(x_2)]\}\rangle_0&=\exp[-k^2aG(x_1-x_2)/2],\\ \langle[\mathbf{r}(x_1)-\mathbf{r}(x_2)]^2\rangle_0&=daG(x_1-x_2)\sim|x_1-x_2|^{2-D},\end{aligned} \quad (2)$$

where

$$\langle\psi\rangle_0=\frac{\int\mathcal{D}[\mathbf{r}(x)]\psi\exp\left[-\frac{1}{2a}\int d^Dx[\nabla\mathbf{r}(x)]^2\right]}{\int\mathcal{D}[\mathbf{r}(x)]\exp\left[-\frac{1}{2a}\int d^Dx[\nabla\mathbf{r}(x)]^2\right]}$$

and $G(x)$ is the Coulomb potential in D space, $|x|^{2-D}/[S_D(2-D)/2]$ with $S_D=2\pi^{D/2}/\Gamma(D/2)$ being the unit-sphere area in D dimensions.

Using the Hubbard-Stratonovich transformation, (1) can be rewritten as

$$\mathcal{P}(\{\mathbf{r}_\alpha\})=\mathcal{N}^{-1}\int\mathcal{D}\phi\,\mathcal{P}(\phi,\{\mathbf{r}_\alpha\}), \quad (3)$$

where

$$\mathcal{P}(\phi,\{\mathbf{r}_\alpha\})=\exp(-H),$$

$$H=\sum_\alpha\left[\frac{1}{2a}\int d^Dx_\alpha[\nabla\mathbf{r}_\alpha(x_\alpha)]^2+i\int d^Dx_\alpha\phi[\mathbf{r}_\alpha(x_\alpha)]\right]+\frac{1}{2w}\int d^dr\,\phi^2(\mathbf{r}),$$

$$\mathcal{N}=\int\mathcal{D}\phi\exp\left[-\frac{1}{2w}\int d^dr\,\phi^2(\mathbf{r})\right].$$

Since the exact calculation of (3) is impossible, I perform a variational calculation seeking a trial Hamiltonian. Due to the presence of other manifolds, we expect the bare interaction $w\delta(\mathbf{r})$ in a labeled manifold to be modified to an unknown interaction $\Delta(\mathbf{r})$, so that $\langle\phi(\mathbf{r})\phi(\mathbf{r}')\rangle=\Delta(\mathbf{r}-\mathbf{r}')$ where the average is done using

(3). As a consequence of Δ, the results of (2) for the labeled manifold are altered and exact results are yet unknown even for the case of $D=1$. Here I assume that Δ leads to the effective Gaussian distribution,

$$\exp\left[-\tfrac{1}{2}\int d^Dx\, a_1^{-1}[\nabla \mathbf{r}(x)]^2\right],$$

where a_1^{-1} is the renormalized elastic constant. In general a_1 is a complicated function of D; however, if we consider (see below) the behavior at large length scales $|x_1-x_2|$ compared to a, we expect a_1 to depend on $|x_1-x_2|$ as a power since the expansion ratio[5] $a_1/a \sim |x_1-x_2|^{2\nu-2+D}$. Therefore, I use the trial probability distribution,[8]

$$\hat{\mathcal{P}}(\phi,\{\mathbf{r}_\alpha\})=\exp(-\hat{H}),$$
$$\hat{H}=\tfrac{1}{2}\sum_\alpha \int d^Dx_\alpha a_1^{-1}[\nabla \mathbf{r}_\alpha(x_\alpha)]^2 + \tfrac{1}{2}\int d^dr \int d^dr' \phi(\mathbf{r})\Delta^{-1}(\mathbf{r},\mathbf{r}')\phi(\mathbf{r}'), \tag{4}$$

where Δ^{-1} is defined by

$$\int d^dr' \Delta^{-1}(\mathbf{r},\mathbf{r}')\Delta(\mathbf{r}'-\mathbf{r}'')=\delta(\mathbf{r}-\mathbf{r}'').$$

Δ and a_1 are determined below.

The probability distribution for a manifold with Δ interaction is given by

$$\mathcal{Y}(\{\mathbf{r}_q\})=\exp\left[-\tfrac{1}{2}\int \frac{d^Dq}{(2\pi)^D}\frac{r_q^2}{g_0(q)} - \tfrac{1}{2}\int d^Dx \int d^Dx' \int \frac{d^dk}{(2\pi)^d}\Delta_k \exp\left[i\mathbf{k}\cdot\int \frac{d^Dq}{(2\pi)^D}\mathbf{r}_q(e^{i\mathbf{q}\cdot\mathbf{x}}-e^{i\mathbf{q}\cdot\mathbf{x}'})\right]\right], \tag{5}$$

where

$$\mathbf{r}(x)=\int \frac{d^Dq}{(2\pi)^D}\mathbf{r}_q \exp(i\mathbf{q}\cdot\mathbf{x})$$

and $g_0(q)=a/q^2$. Δ_k is the d-dimensional Fourier transform of $\Delta(\mathbf{r})$. Adding and subtracting the trial term $\frac{1}{2}\int [d^Dq/(2\pi)^D][r_q^2/g(q)]$ with $g(q)\equiv a_1(q)/q^2$ in the exponent of (5) we get

$$\mathcal{Y}(\{\mathbf{r}_q\})=\exp\left[-\tfrac{1}{2}\int \frac{d^Dq}{(2\pi)^D}\frac{r_q^2}{g(q)} - y(g,\Delta,\{\mathbf{r}_q\})\right],$$
$$y=\tfrac{1}{2}\int \frac{d^Dq}{(2\pi)^D}\left[\frac{1}{g_0(q)}-\frac{1}{g(q)}\right]r_q^2+\frac{w}{2}\int d^Dx \int d^Dx' \int \frac{d^dk}{(2\pi)^d}\Delta_k \exp\{i\mathbf{k}\cdot[\mathbf{r}(x)-\mathbf{r}(x')]\}. \tag{6}$$

Thus the entropy S of one manifold is

$$\frac{S}{k_B}=\ln\int \prod_q d^dr_q \mathcal{Y}(\{\mathbf{r}_q\}) \ge \ln\left[\int \prod_q d^dr_q \exp\left[-\tfrac{1}{2}\int \frac{d^Dq}{(2\pi)^D}\frac{r_q^2}{g(q)}\right]\right] - \langle y\rangle_g,$$

where k_B is Boltzmann's constant and

$$\langle y\rangle_g=\int \prod_q d^dr_q\, y \exp\left[-\tfrac{1}{2}\int \frac{d^Dq}{(2\pi)^D}\frac{r_q^2}{g(q)}\right] \Big/ \int \prod_q d^dr_q \exp\left[-\tfrac{1}{2}\int \frac{d^Dq}{(2\pi)^D}\frac{r_q^2}{g(q)}\right].$$

At the extremum, $\delta S/\delta g=0$ gives

$$dq^2X^D\left[\frac{1}{a}-\frac{1}{a_1}\right]=\tfrac{1}{2}\int d^Dx_1 \int d^Dx_2 \int \frac{d^dk}{(2\pi)^d}k^2\Delta_k \sin^2\left[\frac{\mathbf{q}\cdot(\mathbf{x}_1-\mathbf{x}_2)}{2}\right]\langle e^{i\mathbf{k}\cdot[\mathbf{r}(x_1)-\mathbf{r}(x_2)]}\rangle_g, \tag{7}$$

where X is a typical size of $\mathcal{V}$ and X^D is the internal D-dimensional volume of $\mathcal{V}$. Assuming that the q dependence of a_1 is dominated by small q (large $|x_1-x_2|$) and expanding the right-hand side of (7) in q to $O(q^2)$, (7) becomes for an isolated SA manifold ($\Delta_k=w$)

$$\left[\frac{a_1}{a}\right]^{d/2}\left[\frac{a_1}{a}-1\right]=c_1 z,$$
$$c_1=(2-D)S_D^3\left[1-4\Gamma\left[\frac{D+3}{2}\right]\Big/D(D+1)\Gamma\left[\frac{D-1}{2}\right]\right]\Big/2\epsilon(2D+\epsilon), \tag{8}$$
$$z=[S_D(2-D)/4\pi a]^{d/2}wX^{\epsilon/2},\quad \epsilon=4D-(2-D)d.$$

For small values of z, (8) leads to

$$\langle [\mathbf{r}(x_1)-\mathbf{r}(x_2)]^2\rangle = daG(x_1-x_2)(a_1/a)\ ,$$
$$a_1/a = 1+c_1z+O(z^2)\ , \tag{9}$$

where c_1 is the exact value[9] for $D=1$. For $z\rightarrow\infty$, it follows from (2) and (8) that

$$\langle [\mathbf{r}(x_1)-\mathbf{r}(x_2)]^2\rangle \sim |x_1-x_2|^{2\nu(D,d)}\ , \tag{10}$$

with $\nu(D,d)=(D+2)/(d+2)$ being the Flory exponent.[3,10] Equation (8) is an approximate crossover formula[11] between (9) and (10).

Calculation of Δ. Δ_k is given by

$$\Delta_k = \langle \phi_{\mathbf{k}}\phi_{-\mathbf{k}}\rangle = \int \mathcal{D}[\mathbf{r}]\mathcal{D}\phi\, \phi_{\mathbf{k}}\phi_{-\mathbf{k}}\mathcal{P}(\phi,\{\mathbf{r}_\alpha\}) \Big/ \int \mathcal{D}[\mathbf{r}]\mathcal{D}\phi\, \mathcal{P}(\phi,\{\mathbf{r}_\alpha\})\ . \tag{11}$$

Adding and subtracting $\hat{H}$ of (4) in (3),

$$\mathcal{P}(\phi,\{\mathbf{r}_\alpha\}) = \hat{\mathcal{P}}(\phi,\{\mathbf{r}_\alpha\})\exp[-(H-\hat{H})]\ .$$

Using $\hat{\mathcal{P}}$ as the propagator and expanding $\exp[-(H-\hat{H})]$ in (11), a perturbation theory is constructed.[8] The leading term of this series in Δ_k. Making all terms of the series except the leading term vanish provides a constraint which determines Δ_k,

$$\int \mathcal{D}\phi\, \phi_{\mathbf{k}}\phi_{-\mathbf{k}} \left[\int \frac{d^d\mu}{(2\pi)^d}\phi_\mu \left[\frac{1}{2w} - \frac{\Delta_\mu^{-1}}{2}\right]\phi_{-\mu} - \left\langle \sum_{j=1}^{\infty} \frac{(iH')^{2j}}{(2j)!}\right\rangle_x \right] \times \exp\left[-\tfrac{1}{2}\int \frac{d^dp}{(2\pi)^d}\phi_{\mathbf{p}}\Delta_{\mathbf{p}}^{-1}\phi_{\mathbf{p}}\right] = 0\ , \tag{12}$$

where

$$H' = \sum_{\alpha=1}^{N} \int d^Dx_\alpha \int \frac{d^dk}{(2\pi)^d}\phi_{\mathbf{k}}\exp[i\mathbf{k}\cdot\mathbf{r}_\alpha(x_\alpha)]\ .$$

The subscript x on the angular brackets indicates the averaging over manifold configurations. Denoting $\langle\ \rangle_x$ of (12) by

$$[\rho/2(2\pi)^d]\int d^d\mu\phi_\mu\zeta_\mu\phi_{-\mu}\ ,$$

where $\rho\equiv NX^D/V$ is the manifold density (number of monomers per volume), gives

$$\Delta_\mu = w/(1+w\rho\zeta_\mu)\ . \tag{13}$$

Averaging over the configurations of the manifolds and allowing the center of mass of each manifold to be anywhere inside the volume V of d space, the leading term of $\rho\zeta_\mu$ becomes

$$(N/V)\int d^Dx_1\int d^Dx_2\langle \exp\{i\mu\cdot[\mathbf{r}(x_1)-\mathbf{r}(x_2)]\}\rangle_x\ .$$

For the typical size X of $\mathcal{V}$ very large, this approximates to $A_DX^D(\mu^2a_1)^{-D/(2-D)}$ with

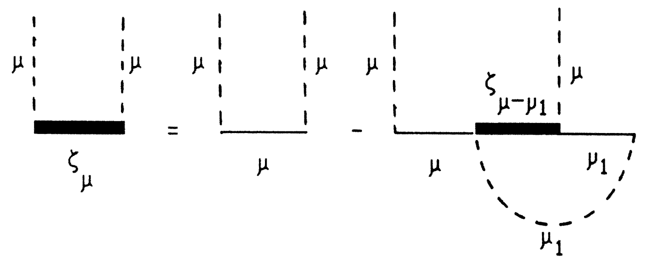
$$A_D = \Gamma[D/(2-D)][S_D(2-D)^{D-1}]^{2/(2-D)}$$

and it follows from (13) that

$$\Delta_k = w/[1+(k^2\xi^2)^{-D/(2-D)}]\ , \tag{14}$$

$$\xi = a_1^{1/2}(A_D\rho w)^{(D-2)/2D} \equiv \xi_E\ . \tag{15}$$

Thus the δ-function interaction is screened and ξ_E is the generalized Edwards screening length.[6,10] The mean-field result of (15) is a consequence of truncating the series of ζ_μ of (12) at the first term. The terms of ζ_μ can be written[8] as the Dyson equation



(16)

Since we are interested in large volumes X^D of the manifold and large distance ($\mu\rightarrow 0$), (16) becomes in this limit,

$$w\rho\zeta_\mu \equiv (\mu\xi)^{-2D/(2-D)} = \frac{w\rho A_D}{(\mu^2a_1)^{D/(2-D)}} - \frac{\beta w A_D^2}{(\mu^2a_1)^{D/(2-D)}}\int \frac{d^dp}{(2\pi)^d}\frac{[1+(p\xi)^{-2D/(2-D)}]^{-1}}{(p\xi)^{2D/(2-D)}(p^2a_1)^{D/(2-D)}}\ , \tag{17}$$

where β is a numerical factor to account for the combinatorial front factors of various diagrams. Therefore ξ is given by

$$\xi^{-2D/(2-D)} = A_Dw\rho/[a_1^{D/(2-D)} + b(D,d)w\xi^{\epsilon/(2-D)}a_1^{-D/(2-D)}]\ , \tag{18}$$

where the coefficient $b(D,d)$ is proportional to β. The unknown a_1 can be determined by substituting (14) into (7). In the limit of $X^D \to \infty$ for a finite ξ corresponding to the situation where the manifolds are interpenetrating

$$a_1^{(D+2)/(2-D)}\left[\frac{1}{a}-\frac{1}{a_1}\right]=b_1(D,d)w\xi^{\epsilon/(2-D)} , \qquad (19)$$

where $b_1(D,d)$ is a numerical coefficient related to c_1. Equations (18) and (19) provide the necessary formulas for the density dependence of ξ and the expansion ratio a_1/a. For the "semidilute" condition (Ref. 10), where ρ is small but large enough to make the manifolds interpenetrating, (18) and (19) give the scaling laws

$$\begin{aligned} &\xi \sim \rho^{-(D+2)/2(d-D)} , \\ &\langle [\mathbf{r}(x_1)-\mathbf{r}(x_2)]^2\rangle \sim |x_1-x_2|^{2-D}\rho^{-\epsilon/2(d-D)} . \end{aligned} \qquad (20)$$

In the large-ρ limit, (18) and (19) yield $\xi \sim \rho^{(D-2)/2D}$ and $a_1=a$ [same result as (15)]. These results are, of course, valid for $d>d^*=2D/(2-D)$ which is the relevant lower critical dimension.

Since we have now established that the bare interaction is screened as the manifold density increases, the results of (20) can be obtained using the following scaling argument. For an isolated manifold $\langle [\mathbf{r}(X)-\mathbf{r}(0)]^2\rangle \sim X^{2\nu(D,d)}$, but for high densities the exponent is changed to $2-D$ due to screening. Hence the density dependence can be written as $X^{2\nu(D,d)}f(\rho/\rho^*)$, where f is a scaling function and ρ is made dimensionless using the overlap density $\rho^* \sim X^{D-d\nu(D,d)}$. Assuming that $f(y)$ is a power law and requiring that X^{2-D} is recovered at high ρ, (20) is obtained. Similarly, since $\xi \sim X^{\nu(D,d)}$ for very low densities, ξ can be written as

$$\xi(\rho) \sim X^{\nu(D,d)} f_1(\rho X^{d\nu(D,d)-D}) .$$

Assuming $f_1(y)$ to be a power of y and requiring that ξ is independent of X at high ρ, (20) is recovered. In an analogous manner the osmotic pressure of the system can be shown to be proportional to $\rho^{d(D+2)/2(d-D)}$.

Using the Feynmann variational procedure, I have demonstrated that SA interaction between multiple points of a manifold is screened due to the presence of other manifolds. As a consequence, the mean-square distance between two points of a labeled manifold decreases to the Gaussian result as the manifold density increases. The derived exponents for the density dependence of the correlation length and the mean-square distance between two points of a manifold are in accord with scaling arguments at low densities and the generalized Edwards mean-field result at high densities.

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