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LETTER TO THE EDITOR

Self-consistent solution for the self-avoiding walk

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Abstract. An improved solution is obtained to Edwards' self-consistent field formulation of the self-avoiding walk problem, and the dominant part of the solution is shown to be self-consistent. The asymptotic form of the mean-square end-to-end separation of the walk is obtained. The results are compared with those of a recent analysis based on renormalization group techniques.

The self-avoiding walk (SAW) appears in theoretical studies of critical phenomena in lattice models and the dimensions of long polymers. There are very few exact results for the SAW; most information comes from numerical work on lattice models (Domb 1969). Theories which treat the self-interaction as a perturbation appear to be unsatisfactory (Domb and Joyce 1972).

Flory (1949) introduced a self-consistent field (SCF) theory for the polymer and obtained an approximate solution (not shown to be self-consistent). Flory's mean-field approximation to the SCF predicts that $\langle \boldsymbol{R}^2 \rangle$, the mean-square end separation of a walk of length L in d dimensions, has the asymptotic behaviour $L^{2\nu}$, where $\nu = 3/(d+2)$ for $1 < d < 4$ and $\nu = \frac{1}{2}$ for $d > 4$ (Fisher 1966, 1969). Edwards (1965, 1967) introduced a more sophisticated version of the SCF theory, based on the method of functional integration, which reproduced the 'Flory result'. His assumptions were not clearly set forth, several mathematical approximations were not assessed, and the question of self-consistency was not raised. Subsequently the formal structure of Edwards' theory was worked out; the coupled Hartree equations were derived, and the importance of the symmetry of the mean field was pointed out (Freed 1971, 1972a).

This letter reports a solution to the formal theory of Edwards. The dominant part of the solution is shown to be self-consistent. The Flory result is recovered, and the nature of the approach to the asymptotic limit is elucidated. A fuller account of these results will be presented elsewhere (Gillis 1973, Gillis and Freed 1974).

The SAW is represented as a diffusion path (continuous random walk) $\boldsymbol{r}(s)$, $0 \leqslant s \leqslant L$, with the 'self-avoiding' interaction $V[\boldsymbol{r}(s)-\boldsymbol{r}(s')]$ between any pair of points along the walk (Edwards 1965, 1967, Freed 1971, 1972a). The number of walks which end at $\boldsymbol{R}$ having started at $\boldsymbol{0}$, denoted by $G(\boldsymbol{R}\boldsymbol{0}; L0)$, is the average of the functional $\exp(-\int_0^L\int_0^L \mathrm{d}s\,\mathrm{d}s' V[\boldsymbol{r}(s)-\boldsymbol{r}(s')])$ over all diffusion paths which end at $\boldsymbol{r}(L) = \boldsymbol{R}$, ie the integral of this functional with the conditional Wiener measure (Gel'fand and Yaglom 1960). This functional integral represents a hierarchy of Green functions instead of the

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usual closed diffusion equation (Freed 1971, 1972a). The hierarchy is closed by applying a functional version of the method of random fields familiar in the infinite-range Ising model (Edwards 1965, 1967, Freed 1971, 1972a). This closure shows that

$$G(\mathbf{R0}; L0) = \langle \mathfrak{G}(\mathbf{R0}; L0[\phi]) \rangle_{\phi}$$

where $\mathfrak{G}[\phi]$ is the causal Green function for a closed diffusion equation with the field $\phi(\boldsymbol{R})$. Evaluating this average over random fields by steepest descents in function space gives the approximation that $G \simeq \mathfrak{G}[\phi_0]$ and an equation for the saddle-point ϕ_0. Thus the coupled equations

$$\left(\frac{\partial}{\partial s} - \frac{l}{6}\nabla^2 + \mathrm{i}\phi_0(\boldsymbol{R})\right)\mathfrak{G}(\boldsymbol{Rr}; ss'[\phi_0]) = \delta(\boldsymbol{R}-\boldsymbol{r})\delta(s-s') \tag{1}$$

$$\mathrm{i}\phi_0(\boldsymbol{r}; L) = \int_0^L \mathrm{d}s' \int \mathrm{d}\boldsymbol{R}' V(\boldsymbol{r}-\boldsymbol{R}')\mathfrak{G}(\boldsymbol{RR}'; s-s'[\phi_0])\mathfrak{G}(\boldsymbol{R}'\mathbf{0}; s0[\phi_0])[\mathfrak{G}(\boldsymbol{Rr}; ss'[\phi_0])]^{-1} \tag{2}$$

represent the formal SCF theory to be solved (Freed 1971, 1972a). The right-hand side of (2) is just $\int \mathrm{d}\boldsymbol{R}' V(\boldsymbol{r}-\boldsymbol{R}')\rho(\boldsymbol{R}')$, where $\rho(\boldsymbol{R}')$ is the density of walks at $\boldsymbol{R}'$, so (1) and (2) represent the usual Hartree-type SCF theory. (l is the effective step length of the walk (Freed 1971, 1972a).) It is clear from (2) that the effective field at any space point $\boldsymbol{r}$ depends on L and on the point $\boldsymbol{R} \equiv \boldsymbol{r}(L)$. Therefore, in general the effective field will have ellipsoidal symmetry, with the foci at $\mathbf{0}$ and $\boldsymbol{R}$.

It is convenient to reformulate the SCF theory in E space, where E is the variable conjugate to L (Freed 1972b). The average over fields can be written in terms of an eigenfunction expansion for $\mathfrak{G}[\phi]$

$$G(\boldsymbol{R}\mathbf{0}; L0) = \int_0^{\infty} \mathrm{d}E\rho(E)\exp(-EL)\langle\psi(\boldsymbol{R}; E[\phi])\psi^{+}(\mathbf{0}; E[\phi])\rangle_{\phi}, \tag{3}$$

where $\rho[E]$ is the density of states and the eigenfunctions ψ satisfy

$$\left(-\frac{l}{6}\nabla^2 + \mathrm{i}\phi(\boldsymbol{r}) - E\right)\psi(\boldsymbol{r}; E[\phi]) = 0. \tag{4}$$

Steepest descents evaluation of $\langle\psi[\phi]\psi^{+}[\phi]\rangle_{\phi}$ in (3) leads to

$$\frac{4\pi l^2}{v}\mathrm{i}\phi_0(\boldsymbol{r}; E) = \left(\frac{\mathscr{G}(\boldsymbol{Rr}; E[\phi_0])}{\psi(\boldsymbol{R}; E[\phi_0])} + \frac{\mathscr{G}(\boldsymbol{r}\mathbf{0}; E[\phi_0])}{\psi(\mathbf{0}; E[\phi_0])}\right)\psi(\boldsymbol{r}; E[\phi_0]), \tag{5}$$

coupled with (4) for $\psi[\phi_0]$ and $(-\frac{1}{6}l\nabla^2 + \mathrm{i}\phi_0 - E)\mathscr{G}[\phi_0] = \delta(\boldsymbol{r}-\boldsymbol{r}')$. (In obtaining both (5) and (2) the usual replacement $V(\boldsymbol{r}-\boldsymbol{r}') \to v\delta(\boldsymbol{r}-\boldsymbol{r}')$, which corresponds to using a soft self-avoiding interaction, was made (Freed 1971, 1972a).)

An approximate expression for $\mathrm{i}\phi_0$ can be obtained from the formal theory. It can then be used to start an iterative solution to (4) and (5) and to (1) and (2). The procedure is to postulate an explicit but approximate functional solution $\tilde{\psi}[\phi]$ to (4), eg, WKB functions, put this $\tilde{\psi}[\phi]$ into (3), and then do the steepest descents to find an explicit but approximate equation for the 'saddle-point' $\mathrm{i}\phi_0$. Then $\mathrm{i}\phi_0$ can be used directly in (4) to construct $\tilde{\psi}[\tilde{\phi}_0]$ and $\mathfrak{G}[\tilde{\phi}_0]$. Finally, these are put into (5). If the right-hand side gives back the $\mathrm{i}\tilde{\phi}_0$ found by steepest descents, the theory is self-consistent. This program can be carried out analytically in terms of WKB functions only for cases where (4) is separable to one-dimensional motions. Thus the general case (ellipsoidal symmetry) does not yield to solution in this manner. Henceforth, the discussion is restricted to a closed walk ($\mathbf{R} \equiv \mathbf{0}$), for which the effective field is spherical.

Since physical arguments (Edwards 1965, 1967) indicate that $i\phi_0(\mathbf{r}; E)$ is a non-negative, monotonically decreasing function of r, only the 's waves' contribute to (5). The latter $\tilde{\psi}[\phi]$ can be written as (Abramowitz and Stegun 1964):

$$\tilde{\psi}(\mathbf{r}; E[\phi]) \simeq \frac{1}{(2\pi)^{1/2} r}\left(\frac{w(r; E[\phi])}{p^2(r; E[\phi])}\right)^{1/4} \mathrm{Ai}(-w), \tag{6}$$

$$\tfrac{2}{3}w^{3/2} \equiv \int_r^{r_t} \mathrm{d}r' \left[\frac{6}{l}\left(i\phi(r') - \frac{l}{24r'^2} - E\right)\right]^{1/2} \equiv \int_r^{r_t} \mathrm{d}r' p(r'; E[\phi]). \tag{7}$$

Here Ai is the Airy function, which represents the uniform semi-classical approximation that is free from the divergences which plague WKB functions at turning points. r_t is the 'classical turning point', at which $p(r'; E[\phi]) = 0$. Putting (6) with $\mathbf{R} \equiv \mathbf{0}$ into (3) and doing the steepest descents gives the saddle-point equation

$$\frac{4\pi l^2}{v^2} i\phi_0(r; E) = \theta(r_t - r)\left[\frac{6}{l}\left(i\phi_0 + \frac{l}{24r^2} - E\right)\right]^{1/2}, \tag{8}$$

where θ is the usual step function (Freed 1972b). For $r \lesssim l$, (8) has the dominant solution $i\phi_0 \propto r^{-1}$, which is the same as for the purely random walk (Edwards 1965, 1967). This happens here because the Wiener measure is inappropriate for short walks. Therefore, the SCF theory is poor for short distances. For $l \lesssim r < r_t$, the 'Langer correction' $l/24r^2$ can be dropped (Messiah 1959). Then $\Omega \equiv i\phi_0/E$ satisfies the equation

$$\Omega^3 - \Omega^2 + \frac{\gamma^3}{E^3 r^4} = 0, \tag{9}$$

where $\gamma \equiv (v/4\pi l^2)^2 6/l$ and $r_t \to \infty$. Thus Ω is a function only of the dimensionless parameter $Er^{4/3}\gamma^{-1}$. As $E \to 0$, the one real, positive root of (9) goes as $\gamma r^{-4/3}$. (Edwards found this $E = 0$ solution for (1) and (2) from an integral equation (Edwards 1965, 1967).)

To demonstrate self-consistency of the leading term in the solution, it is sufficient to use $i\phi_0 \sim \gamma r^{-4/3}$ in (4) as proposed above. Finally, the right-hand side of (5) gives back

$$i\phi_0(r; E) = \gamma r^{-4/3}[1 + O(r^{1/3})]. \tag{10}$$

The leading term in the solution is therefore self-consistent. Furthermore, $\gamma r^{-4/3}$ can be used in (1) and (2) in a similar way to show that

$$i\phi_0(r; L) \propto r^{-4/3}[1 + O(r^{1/3})]. \tag{11}$$

This also demonstrates the self-consistency of the leading term in Edwards' theory (1) and (2) (Edwards 1965, 1967).

In (2) and (5), Green functions appear which refer to only a part of the walk. They satisfy (1) and (4) with the same $i\phi_0$ which determines the Green function for the entire walk. Therefore, to the extent that an open walk can be represented as a piece of long closed loop, its Green function can be approximated by a solution of (1) or (4) with the mean field from (5)†. In d dimensions, the leading term in the field is $r^{-2(d-1)/3}$. For $d > 4$, it is more singular than r^{-2} as $r \to 0$, and the walk cannot return to the origin. This is consistent with Rubin's observation (Rubin 1953) that for $d > 4$ diffusion paths are self-intersecting only on a set of measure zero, and hence that $v = \frac{1}{2}$ for $d > 4$. In

† The justification for the consideration of part of a long closed loop has been given by des Cloiseaux (1970).

d (<4) dimensions, Ω is a function only of the dimensionless variable $z \equiv \alpha r E^{3(d-1)/2}$, where α is a constant. For $r \simeq r_t$, the Langer correction is negligible in the 'action integral' in (7). Then the integral is a function only of z. This shows that $\psi_d(R; E)\psi^+(0; E)$ constructed from (4) with the spherical mean field depends on R only through z. It can then be shown (by steepest descents integration as $L \to \infty$) that

$$\mathfrak{G}_d(R0; L0[\phi_0]) = \int \mathrm{d}E \rho(E) \exp(-EL)\psi_d(R; E[\phi])\psi_d^+(0; E[\phi])$$

is a function of R only through the dimensionless variable $\beta R L^{-3/(2+d)}$, where β is another constant. This implies the Flory result. Corrections to this asymptotic dependence can be worked out explicitly for $d = 2, 3$; they are consistent with

$$\langle \boldsymbol{R}^2 \rangle \propto L^{6/(2+d)}[1 + \lambda_1(d)L^{-(4-d)/(2+d)} + \lambda_2(d)L^{-2(4-d)/(2+d)} + \ldots] \qquad 1 < d < 4. \quad (12)$$

De Gennes (1972) found that the ϵ expansions for ν found by the Wilson method and from the Flory result had different coefficients in first order. The meaning of this discrepancy is not yet clear. The Flory result gives an explicit function $\nu_F(\epsilon)$, whereas the Wilson expansion may not represent ν exactly, since $\nu(\epsilon)$ may not be a branch of an analytic function (J des Cloiseaux, private communication).

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