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LETTER TO THE EDITOR

A stochastic quantisation study of the Edwards Hamiltonian

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Abstract. We study the Edwards model of polymer physics using techniques based on stochastic quantisation. The approximating theory with dimensionless coupling constant is conjectured to have end-to-end distance given exactly by the Flory formula.

This letter is a preliminary study of the Edwards model based on stochastic quantisation, using the techniques introduced by Alfaro *et al* (1985). We note that the Edwards model (Edwards 1965) is a model of a single polymer in a good solvent, as well as being one of the simplest examples of quantum field theories. More precisely, by the Edwards model we mean the equilibrium statistical mechanical theory with the Hamiltonian

$$H = H_0 + H_{\text{int}}$$

where

$$H_0 = \tfrac{1}{2}\int_0^{N_0} (\dot{c}(\tau))^2 \, d\tau$$

$$H_{\text{int}} - \tfrac{1}{2}v_0 \int_0^{N_0} d\tau \int_0^{N_0} ds\, \delta(c(\tau) - c(s)).$$

($c(\tau)$ is a vector valued function describing the position of the τth monomer and small contour length cut-off is implicit.)

To study this model via the method of Alfaro *et al* we study the limit, as the time goes to infinity, of the following stochastic process (the 'stochastic Edwards model')

$$\partial c(t, \tau)/\partial t = f(t, \tau) - \delta H/\delta c(t, \tau)$$

where H is as defined previously and $f(t, \tau)$ is a Gaussian noise with zero mean and

$$\langle f^\alpha(t, s) f^\beta(t', s')\rangle = 2\delta_{\alpha\beta}\sigma/2|t - t'|^{\sigma-1}\delta(s - s').$$

Note that in the limit $\sigma \to 0$ the noise becomes delta correlated (for σ approaching 0 from above). We then let $\sigma \to 0$ and (presumably) recover the equilibrium statistics of the Edwards model.

As the first step in this programme we study the stochastic Edwards model with $H = H_0$ only. We choose to study the correlation function

$$C \equiv \lim_{t\to\infty} \langle (c(t, N_0) - c(t, 0))^2\rangle$$

for finite $\sigma > 0$ and use the Green function

$$G(t, t', \tau, \tau') = \theta(t - t')1/N_0\left\{-1 + 2\sum_{p=0}^{\infty} \cos\left(\frac{\pi p}{N_0\tau}\right)\cos\left(\frac{\pi p}{N_0\tau'}\right)\exp\left[-\left(\frac{\pi p}{N_0}\right)^2(t - t')\right]\right\}$$

corresponding to force-free end conditions (Schaub *et al* 1985). An easy calculation yields

$$C = 2dN_0^{1+2\sigma} \sum_{p=1}^{\infty} (1/\pi p)^{2+2\sigma}\Gamma(1+\sigma)[-1+(-1)^p]^2$$

(d is the spatial dimension).

Note that in the limit $\sigma \to 0$ we recover the standard equilibrium result $\langle (c(N)-c(0))^2\rangle = dN_0$. We also observe that if $\sigma < 0$ we encounter divergent integrals in the calculation of C.

To proceed with the interacting theory we find a value of σ, σ^* where the coupling constant v_0 is dimensionless. Assigning the time t a dimension L we find the dimension of $v_0 = L^\alpha$ where

$$\alpha = \sigma - 1 + d\sigma/2 + d/4$$

and so

$$\sigma^* = (1-d/4)/(1+d/2).$$

Combining this with the free calculation of the end-to-end distance we find that for $\sigma = \sigma^*$ the end-to-end distance goes as $N_0^{2\nu}$ where $\nu = 3/(2+d)$. We recognise the formula for the end-to-end distance exponent as the Flory formula (de Gennes 1980). Because $\sigma = \sigma^*$ is the 'value' of the noise for which the coupling constant is dimensionless, and the value of σ for which the theory is presumably renormalisable, we conjecture that for the (renormalised) interacting theory at $\sigma = \sigma^*$ the end-to-end distance molecular weight dependence is given by the Flory formula (to leading order in N). It appears that an expansion in σ around $\sigma = \sigma^*$ is an expansion around a theory for which the Flory exponent is exact.

It is also interesting to note that the values of σ^* for which the stochastic Edwards model has a dimensionless coupling constant are different from the corresponding values of σ^* in the stochastic O(M) model (in the O(M) model $\sigma^* = -2 + (d/2)$). It thus appears there is no simple relationship between the stochastic O(M) models at $\sigma \neq 0$ and the stochastic Edwards model. (The Edwards model is the $M \to 0$ limit of the O(M) model (de Gennes 1972).)

Moreover, dimensional analysis indicates that the stochastic Edwards model is better behaved (for $d<4$) since σ^* for an O(M) model is negative while for the stochastic Edwards model σ^* is positive. (For example for $d=3$ $\sigma^*(\mathrm{O}(M)) = -\frac{1}{2}$ while σ^* (Edwards) $= \frac{1}{10}$.) It has been suggested that noise being negatively correlated at small times indicates pathological behaviour (Damgaard 1986). (We also note that

$$\lim_{\sigma \to 0} \sigma/2t^{\sigma-1} = \delta(t)$$

is true only if σ approaches 0 through positive values.)

We have attempted to substantiate the above conjectures (the renormalisability of the theory at $\sigma = \sigma^*$ and the N dependence of $\langle R^2\rangle$) by performing a bare perturbation calculation for σ near σ^* (ultimately hoping to renormalise the theory and extract the critical exponents for σ near σ^* by renormalisation group arguments). Unfortunately at finite N_0 such calculations proved to be rather difficult. We have thus considered a stochastic Edwards model for an infinite chain. (In the Hamiltonian replace $\int_0^{N_0}$ by $\int_{-\infty}^{\infty}$; the dimensional analysis is the same as for the finite chain case.) For this model the Green function takes the form

$$G(t, t', \tau, \tau') = 1/(2\pi)\theta(t-t') \int_{-\infty}^{\infty} \exp[\mathrm{i}q(\tau-\tau') - q^2(t-t')]\,\mathrm{d}q$$

and so calculations are simplified. We have calculated to first order in v_0 the correlation function

$$D(\tau, s) \equiv \lim_{t\to\infty} \langle (c(t,\tau) - c(t,s))^2 \rangle$$

for σ slightly less than σ^*. We find that

$$D(\tau, s) = C_1|\tau - s|^{2\sigma+1} + V_0 C_2 |\tau - s|^{4+2\sigma-\alpha}\left(\int_0^\infty \mathrm{d}x \frac{1-\cos x}{x^\alpha}\right)$$
$$\times\left(\int_0^\infty \mathrm{d}w\, w^{\sigma+1}\,\mathrm{e}^{-w}\right)\left(\int_0^\infty \mathrm{d}p \frac{1-\cos p}{p^{5+2\sigma-\alpha}}\right)$$

where

$$\alpha = (2\sigma+1)[(d/2)+1]$$
$$C_1 = \frac{d}{\sqrt{\pi}} \int_0^\infty \mathrm{d}w\, w^{\sigma-1/2}(1 - \mathrm{e}^{-1/4w})$$
$$C_2 = (d/2^{d-1})(1/\pi^{d/2+1})(1/K_1^{d/2+1})$$
$$K_1 = C_1/2d.$$

We see that for σ slightly less than σ^* ($d = 2$ or 3) all integrals are finite and at $\sigma = \sigma^*$ the integral

$$\int_0^\infty \mathrm{d}x(1-\cos x)/x^\alpha$$

diverges logarithmically (while the other integrals remain finite) as expected. Note that the dependence on $|\tau - s|$ is given by dimensional analysis. (The $|\tau - s|$ dependence of the general term of order v_0^n is $|\tau - s|^\beta$ where $\beta = 1 + 2n - nd/2 + \sigma(2 - 2n - nd)$.)

To apply renormalisation group arguments it is necessary to complete the calculation to second order (to determine the renormalisation of the coupling constant (Oono 1985)). Such a calculation appears to be feasible and is currently being undertaken.

An interesting aspect of the method introduced by Alfaro *et al* (1985) is that there are two parameters, σ and the dimension d, which one can vary in the search for a theory where the coupling constant is dimensionless. One would then expect the method to be more versatile than the ε expansion. We are thus motivated to ask the following question: is there a choice of the dimension (not necessarily integral) and noise for which v_0 (introduced earlier) and w_0 are simultaneously dimensionless where w_0 is the coefficient of the three-body force (Oono 1985)

$$H_{\text{int three body}} = w_0/3! \int \mathrm{d}\tau \int \mathrm{d}s_1 \int \mathrm{d}s_2 \delta(c(\tau) - c(s_1))\delta(c(\tau) - c(s_2)).$$

If such a theory exists it could prove to be useful in the study of the theta point. (For another approach see Oono (1984).) By dimensional analysis we find this is never possible except for the choice $d = 1$ and $\sigma = \frac{1}{2}$. (In the analogous case for the $\mathrm{O}(M)$

model this is never possible. It is impossible to find a value of the dimension and the noise where the coefficients of $(\phi\cdot\phi)^2$ and $(\phi\cdot\phi)^3$ are simultaneously dimensionless.) In a sense, this is very natural since for this choice of σ and d the unperturbed chain (H_0 only) has an end-to-end distance proportional to N_0^2 (the chain is fully stretched). It is thus not suprising that dimensional analysis tells us in fact that all the w_n (where w_n is the coefficient of the n-body term) are also dimensionless for $d=1$, $\sigma=\frac{1}{2}$. It is important to note, however, that for the infinite chain, the case $\sigma=\frac{1}{2}$, $d=1$ appears to be ill-defined; even in the unperturbed case when one calculates $D(\tau, s)$ divergent integrals appear.

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