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Short Communication

Force-free motion in an asymmetric environment: a simple model for structured objects

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Abstract. — Recent models have shown how dissipation of energy can set into directed motion a point-like particle in an environment of vectorial symmetry, even in the absence of macroscopic forces. This statement is extended to the case of an object with an internal structure, focusing on the simplest model: an elastic dumb-bell. We briefly show that specific mechanisms then come into play, able to set the object into directed motion even if thermal diffusion is negligible.

1. Introduction.

Recent theoretical works have shown how particles in a periodic environment can be set into motion in the absence of any macroscopic force or gradient provided that: (i) the structure possesses vectorial symmetry, (ii) energy dissipation takes place [1-9]. The latter, granting that the system is maintained out of equilibrium, can manifest itself in various forms, e.g. the variation in time (periodic or stochastic) of the effect of the structure on the particle [1-5, 9] or the presence of a non-white noise acting on the particle [6-8]. These models may be of some relevance to analyze the motion of motor protein assemblies which have the above mentioned symmetry [3-10], but also help designing artificial selective pumping devices for various kinds of objects [11, 12].

However, these models addressed the case of point-like particles described by one spatial degree of freedom \(z\), with in some cases an additional parameter describing the interaction between the particle and its environment, this parameter changing in time periodically [1-3, 9] or stochastically [3-5, 9]. The aim of the present note is to briefly point out that (and how) motion can also result from the internal structure of the object placed in the asymmetric environment.

For this purpose we take the simple model of a "dumb-bell" two point-like particles linked by an elastic spring (an object with a single internal degree of freedom). Focusing on specific regimes, we then show that motion can be obtained due to the presence of the corresponding internal mode in two cases: (A) the object is immersed in a sawtooth potential switched on and off periodically, (B) each of the two particles stochastically undergoes transitions between two states, which results in a variation of its sensitivity to a stable asymmetric environment. In both cases, motion persists in the limit of zero diffusivity of the particles. This feature clearly exhibits the difference between the mechanism described here and those proposed for a single point-like particle under the same conditions [1-6]. The present mechanism is also

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different from that at work in a very recent two-head motor protein model [13], although some ingredients are similar.

2. Model.
We consider the one-dimensional motion along a direction $x$ of an object represented as a “dumb-bell”. two identical particles P1 and P2, interacting with each other through a potential

$$U_{\text{int}} = 1/2K(x_2 - x_1 - \ell_0)^2,$$

(1)

where $x_1$ and $x_2$ are the positions of P1 and P2 respectively ($x_1 > x_2$), and $\ell_0$ gives a measure of the equilibrium size of the object.

To model an environment of vectorial symmetry we will consider a simple periodic sawtooth potential, defined by its value on a period $p$:

$$U_{\text{asym}} = U_0 + W(x/a) \quad \text{for } 0 < x < a$$

$$U_{\text{asym}} = U_0 + W(p-x)/b \quad \text{for } a < x < p,$$

(2)

where $a$, $b = p - a$ are the lengths of the two sides of a “tooth” ($a < b$).

As in previous studies [1-5], we will here focus on two cases:

- case A: the source of the potential $U_{\text{asym}}$ is switched periodically on (during $\tau_{\text{on}}$) and off (during $\tau_{\text{off}}$). So both particles are simultaneously periodically submitted to $U_{\text{asym}}$.

- case B: the source of the potential $U_{\text{asym}}$ is stable but each particle independently undergoes transitions between a state (+) where it feels $U_{\text{asym}}$ and a state (−) where it does not. Life times $\tau_+$ and $\tau_-$ in the two states are taken equal for the two particles and independent of $x$, which implies that some external action has moved the system away from equilibrium and the ratio $\tau_+(x)/\tau_-(x)$ from its detailed balance value $\exp(-U_{\text{asym}}(x)/kT)$ [3].

Introducing the internal structure of the object adds to the preexisting typical scales of energy ($W$ and $kT$), time ($\tau_i$ $(i \in \{+, −, \text{on}, \text{off}\})$), $p^2\xi/kT$ and $p^2\xi/W$, and size ($p$), those related to the internal mode: $K\ell_0^2/\xi/K$, and $\ell_0$ (where $\xi$ is the friction coefficient of the particles).

Solving the complete set of equations corresponding to cases A and B therefore becomes somewhat complicated, and we here restrict the analysis to the following regimes as to exhibit simply mechanisms able to induce motion:

(R1) The energy scale of the potential is taken much larger than that of the interaction between the two particles: $W \gg K\ell_0^2$.
(R2) Thermal diffusion is neglected.
(R3) Relaxation of the internal mode of the object is faster than the time involved in the cycles “particle/asymmetric environment”: $\xi/K \ll \tau_i$.
(R4) Relaxation under the effect of $U_{\text{asym}}$ is also faster: $\xi p^2/W \ll \tau_i$.

(R1), (R2) and (R4) imply that whenever a particle feels $U_{\text{asym}}$ it gets quickly trapped at the bottom of the corresponding valley. (R2) and (R4) imply that whenever (at least) one particle ceases to feel $U_{\text{asym}}$, the dumb-bell relaxes quickly (≈ instantaneously) to its equilibrium size $\ell_0$. Within this frame of hypothesis it is easy to prove that the particle is set into motion provided $\ell_0$ and $(p, a)$ are appropriately chosen.
3. Case A: asymmetric potential applied periodically.

In case A, the sawtooth potential $U_{\text{sym}}$ acts periodically and simultaneously on the two particles. When it is applied $P_1$ and $P_2$ get trapped at the bottom of the valley where they sit. When it is turned off the spring relaxes back symmetrically to $\ell_0$.

A way to get directed motion is that upon retrapping, the dumb-bell gets successively stretched and compressed, and that in some of the resulting relaxation steps, $P_1$ or $P_2$ manages to move to the neighbour valley of $U_{\text{sym}}$. Figure 1 illustrates this by showing the dumb-bell at the end of “on” and “off” periods: net motion towards the right of the picture is clear. This holds because the periodicity and asymmetry of the structure and $\ell_0$ have been chosen in such a way that $p + 2a < \ell_0 < p + (b - a)$, which implies $b > 3a$. More generally, a similar motion is obtained if:

$$np + 2a < \ell_0 < np + (b - a),$$

the dumb-bell cycling between compression ($x_2 - x_1 = np$) and extension ($x_2 - x_1 = (n + 1)p$) at the end of the “on” periods. Under such conditions, the obtained velocity is:

$$V = p/2(\tau_{\text{on}} + \tau_{\text{off}}).$$

This steady state picture is reached whatever the initial conditions. Note also that for this process to be efficient, the object has to be larger than some characteristic size of the environment: $2a < \ell_0$ at least (case $n = 0$).

---

Fig. 1. — Case A. The potential $U_{\text{sym}}$ is represented on top of the picture. (a) to (e). Positions of the dumb-bell at the end of successive on and off periods are exhibited. The dumb-bell has relaxed to its natural length $\ell_0$ in (b) and (d), is extended in (a) and (e), and compressed in (c). It has moved one period to the right of the picture in two consecutive on/off cycles.
4. Case B: two-state model for the particles.

Let us now turn to a picture in which P1 and P2 transit independently between state (+) and (−). Within hypothesis R(3) and R(4) the system generically relaxes between transitions. Therefore, defining $n$ by $np < \ell_0 < (n + 1)p$, the state of the system before one of the particles undergoes a transition belongs to the following list (see also Fig. 2 for the case $n = 1$):

- **A$_1$**: Both particles are in state (+). P1 is trapped at $x_1 = ip$ and P2 is trapped at $x_2 = (i + n + 1)p$. The spring is extended in this state as $x_2 - x_1 > \ell_0$.

- **B$_1$**: Both particles are in state (+). P1 is trapped at $x_1 = ip$ and P2 is trapped at $x_2 = (i + n)p$. The spring is compressed in this state as $x_2 - x_1 < \ell_0$.

- **C$_i^+$**: P1 in state (+) is trapped at $x_1 = ip$ and P2 in state (−) gets to the position that relaxes the dumb-bell: $x_2 = ip + \ell_0$.

- **C$_i^−$**: Both particles are in state (−), $x_1 = ip$ and $x_2 = ip + \ell_0$.

- **D$_i^+$**: P2 in state (+) is trapped at $x_2 = (i + n)p$ and P1 in state (−) gets to the position that relaxes the dumb-bell: $x_1 = (i + n)p - \ell_0$.

- **D$_i^−$**: Both particles are in state (−), $x_1 = (i + n)p - \ell_0$ and $x_2 = (i + n)p$.

![Diagram of Case B](image)

**Fig. 2.** — Case B. The potential $U_{\text{asym}}$ is represented on top of the figure. The six states described in section 4 are displayed for a case where $p + a < \ell_0 < p + b$. Cycling between these states along equation (6) leads to net motion to the right.
Let us consider a dumb-bell such that

\[ np + a < \ell_0 < np + b. \]  

Then, with the help of figure 2, it is easy to see that upon P1 or P2 undergoing a transition, the system moves according to:

\[
\begin{align*}
A_i & \rightarrow D^+_{i+1} \text{ or } C^+; \\
B_i & \rightarrow D^+_i \text{ or } C^+_i; \\
C^+_i & \rightarrow C^-_i \text{ or } A_i; \\
C^-_i & \rightarrow C^+_i \text{ or } D^+_{i+1}; \\
D^+_i & \rightarrow B_i \text{ or } D^-_i; \\
D^-_i & \rightarrow C^+_i \text{ or } D^+_i
\end{align*}
\]  

(6)

It is clear that index \( i \) never regresses and sometimes progresses during stochastic wandering between states along these rules: net motion to the right is obtained.

To get a numerical estimate of the velocity, one can simplify the problem further with the hypothesis that the particles spend most of their time in state \((+): \tau_- \ll \tau_+\), so that typical sequences are P1 (P2) transits to state \((-)\) and then quickly back to \((+)\) before something happens to P2 (P1). In this limit equation (6) reduces to:

\[
\begin{align*}
A_i & \rightarrow B_{i+1} \text{ or } A_i; \\
B_i & \rightarrow B_i \text{ or } A_i
\end{align*}
\]  

(7)

The four corresponding transition rates are equal to \(1/\tau_+\). The object spends half of its time in state \( B \) and half in state \( A \), where the index \( i \) progresses by 1 on average after time \( \tau_+\). The average velocity is thus:

\[ V \approx p/2\tau_. \]  

(8)

5. Discussion.

- Through a very simple model and focusing on given regimes, we have shown that (and how) an object can be set into directed motion in an asymmetric environment, in the absence of macroscopic external forces, provided a certain fit between its internal structure and the environment characteristics (e.g. Eqs. (3) and (5)).

- The deterministic motion obtained here is in the same direction as that predicted for a point-like particle in similar circumstances [2-4], and the resulting average velocities span the same ranges of magnitude (typically a fraction of the period \( p \) per cycle). Note however that the underlying mechanism is structurally different as it survives thermal diffusion going to zero. From this point of view, the present model shares some similarity with that presented in reference [9], in which a point-like particle is successively under the influence of two asymmetric potentials of same period, but with minima spatially shifted by some distance. Here in some sense, the particle carries the analog of a “shift”: its size \( \ell_0 \).

- It is clear that the introduction of thermal diffusion will modify the picture, introducing stochasticity in case A and developing it in case B. Solving in a general way the model of section 2 without restrictions (R1-4) would lead to a frame encompassing both the limit presented here and those of references [2-4] corresponding to \( \ell_0 \ll a \). These more elaborate calculations are needed to determine the conditions leading to optimal velocities or abilities of these motors/pumps to resist external forces. Note that the additional force scale \( K\ell_0 \) introduced in this model should show up in such an analysis.

- On symmetry grounds, one should be able to get motion in a symmetric periodic structure with an asymmetric dumb-bell: P1 and P2 different e.g. in their friction coefficients.
transition rates, etc.. However, this requires thermal diffusion to act, once again similarly to the model of two shifted potentials [9] in the case where the two potentials are chosen symmetric [14]. Note that under such conditions tumbling will stochastically occur (P2 moving to the left of P1), after which the object will start moving in the reverse direction. 

The motion would then appear as directed up to a certain (possibly very long) time scale and random at longer times.

- In a recent more elaborate model [13], Peskin and Oster consider a symmetric two-head motor protein, where the interaction with the polar substrate (microtubule) induces an asymmetry in the “unbinding” transition (somewhat analogous to the present \( + \rightarrow - \) ) rate of the two heads (particles). When one head (particle) unbinds, it can rebind only at one of the neighbour trapping sites of the still attached head: it either rebinds at the position it has just left or binds on the other side of the attached head (the front and back head exchanging their roles). If the “back” head detaches more often than the “front” head, the resulting waltz leads the object to progress “forwards”. This model gives a very good agreement with experimental data for kinesin motors [13]. It relies however on mechanisms somewhat different from those presented here (e.g. diffusional tumbling is permanently at work and trapping occurs only on specific sites).

- Molecular models for biological motor processes [13, 15] could make use of bases similar to those of the present simple model, but we emphasize that the latter may also be a useful guide to develop selective pumping devices sensitive to internal parameters [11, 12].

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References

Manifolds in random media: a variational approach to the spatial probability distribution

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Abstract. — We develop a new variational scheme to approximate the position dependent spatial probability distribution of a zero dimensional manifold in a random medium. This celebrated ‘toy-model’ is associated via a mapping with directed polymers in 1+1 dimension, and also describes features of the commensurate-incommensurate phase transition. It consists of a pointlike ‘interface’ in one dimension subject to a combination of a harmonic potential plus a random potential with long range spatial correlations. The variational approach we develop gives far better results for the tail of the spatial distribution than the Hamiltonian version, developed by Mezard and Parisi, as compared with numerical simulations for a range of temperatures. This is because the variational parameters are determined as functions of position. The replica method is utilized, and solutions for the variational parameters are presented. In this paper we limit ourselves to the replica symmetric solution.

1. Introduction.

Recently a lot of attention has been devoted to the behavior of manifolds in random media [1-21]. This is partially due to their connection with vortex line pinning in high \(T_c\) superconductors [11, 21], but also because of the intrinsic interest in the behavior of interfaces between two coexisting phases of a disordered system, like magnets subject to random fields or random impurities. In addition mappings are known to exist between one dimensional manifolds like directed polymers in disordered media and growth problems in the presence of random noise described by the KPZ equation [22].

The variational method [8, 13, 16] appears to be an important tool in approximating many properties of the system like the calculation of the roughness exponent of a wandering manifold in a disordered medium. Recently we have conducted a numerical study of the spatial probability distribution of directed polymers in 1+1 dimensions in the presence of quenched disorder [15]. Directed polymers refer to an interface in two dimensions with no overhangs. In addition to the width of the interface, it is important to know what is the probability that the interface would wander a certain distance in the transverse direction. We have then exploited a mapping
of this system into that of a pointlike interface in one dimension subjected to a combination of a harmonic restoring force and a random potential with long ranged correlations.

Using that mapping combined with a use of the variational approximation, we were able to derive many properties of the spatial probability distribution (PD) of the directed polymers [16]. In particular the function $f(\alpha)$ associated with the decay of the probability for different realizations of the disorder has been derived using the replica method. Replica symmetry breaking solutions have been used (at low temperatures). The mapping from directed polymers to the so called toy-model is discussed in detail in reference [16] based on previous work by Parisi [5] and Bouchaud and Orland [6]. In particular the spatial probability distribution of directed polymers at large times relates to the spatial probability distribution of the toy-model at low temperature. Villain et al. [1] emphasize directly the relation between the toy-model and the commensurate-incommensurate transition in systems with quenched impurities [1].

Using the replica method the toy-model can be mapped into an $n$-body problem were the interaction between different particles (replicas) is given by the correlation of the original random potential. The variational method utilizes an effective quadratic Hamiltonian whose parameters are chosen by the stationarity method to give a good approximation for the free energy of the $n$-body system in the limit $n \to 0$ [8]. The results it provides for the tail of the spatial distribution are not very accurate as will be shown below (Sect. 4). In this paper we describe a way to directly apply the variational approach to the probability distribution rather than to the Hamiltonian or the free energy. As we shall see it gives a much better approximation for the behavior of the tail of the distribution. For high temperatures the results appear almost exact without the need to break replica symmetry.

2. The variational method applied to the probability distribution.

The toy model [1, 4, 13, 16] involves a classical particle in a one-dimensional potential consisting of a harmonic part and a spatially correlated random part. It is the simple prototype of an interface -- a point in one dimension -- which is localized by a harmonic restoring force, and pinned by quenched impurities the distribution of which may be correlated over large separations. Its Hamiltonian is given by:

$$H(\omega) = \frac{\mu}{2} \omega^2 + V(\omega),$$

(1)

where $\omega$ denotes the position of the particle and $V(\omega)$ is a random potential with a Gaussian distribution characterized by:

$$\langle V(\omega) \rangle = 0, \quad \langle V(\omega)V(\omega') \rangle = -\frac{g}{2(1-\gamma)} |\omega - \omega'|^{2-2\gamma} + \text{Const.} \equiv -f((\omega - \omega')^2),$$

(2)

where the brackets indicate averaging over the random potential. In the sequel without loss of generality we will take the constant on the r.h.s. of equation (2) to be zero. We will make use of the replica method to replicate the partition function

$$Z = \int d\omega \exp(-\beta H)$$

(3)
and average it over the random potential to express it in terms of an effective $n$-body Hamiltonian:

$$
(Z^n) = \int d\omega_1 \ldots d\omega_n \exp(-\beta \mathcal{H}),
$$

$$
\mathcal{H} = \frac{1}{2} \mu \sum_{a=1}^{n} \omega_a^2 + \frac{1}{2} \beta \sum_{ab} f \left( (\omega_a - \omega_b)^2 \right). \quad (4)
$$

For later use let us also define an $n$-body quadratic Hamiltonian:

$$
h = \frac{1}{2} \mu \sum_{a=1}^{n} \omega_a^2 - \frac{1}{2} \beta \sum_{ab} \sigma_{ab} \omega_a \omega_b \quad (5)
$$

where the matrix elements of $\sigma_{ab}$ are free parameters at this point.

We consider cases in which the potential has long-range correlations, (i.e. $\gamma < 1$), and in particular we are interested in the case $\gamma = \frac{1}{2}$ because of the above mentioned mapping from directed polymers in $1+1$ dimensions. Let us review briefly the variational scheme used by Mezard and Parisi. We start with the well known inequality

$$
\langle e^A \rangle \geq e^{\langle A \rangle} \quad (6)
$$

The Mezard-Parisi variational approximation [8] can be obtained from this inequality, by choosing

$$
-\frac{1}{\beta} A(\omega_1, \ldots, \omega_n) = \mathcal{H}(\omega_1, \ldots, \omega_n) - h(\omega_1, \ldots, \omega_n) \quad (7)
$$

And by defining the average as

$$
\langle A \rangle = \frac{\text{Tr} A \exp \left( -\beta h \right)}{\text{Tr} \exp \left( -\beta h \right)}. \quad (8)
$$

with

$$
\text{Tr} = \int_{-\infty}^{+\infty} d\omega_1 \ldots d\omega_n \quad (9)
$$

This yields

$$
nf = -\frac{1}{\beta} \ln \text{Tr} \exp \left( -\beta \mathcal{H} \right) \leq \langle H - h \rangle - \frac{1}{\beta} \ln \text{Tr} \exp \left( -\beta h \right), \quad (10)
$$

where $f$ is the free energy. The variational free energy is given by the right hand side of equation (10) at the point of stationarity. This procedure provides equations for the variational parameters which are the elements of the matrix $\sigma_{ab}$. MP [13] have solved these equations and found a replica symmetric (RS) solution valid for high temperatures and a solution which breaks replica symmetry (RSB) at low temperatures.

Recall that the limit $n \to 0$ has to be taken when making use of the replica method. An important point to bear in mind is that the inequality (6) holds only when $n$ is a positive integer, provided the parametrization of $\sigma$ is such that $\text{Tr} \exp(-\beta h) < \infty$. This is because only in this case the integration measure

$$
\left[ \text{Tr} \exp(-\beta h) \right]^{-1} \exp \left( -\beta h \right) d\omega_1 \ldots d\omega_n, \quad (11)
$$

is a real positive measure on $\mathbb{R}^n$, for which the proof of the inequality (6) holds (see e.g. [23] p. 61). In the limit $n \to 0$ the inequality can change sign and does not hold in general, but one
still expects the stationary point of the r.h.s. of equation (10) to give a good approximation to the l.h.s. i.e. to the exact free energy. Support for this contention comes also from the fact that the variational method becomes exact for a manifold embedded in $d$ spatial dimensions when $d$ becomes infinite, and one can systematically improve it by a $1/d$ expansion [8, 13, 17, 19].

Let us define

$$\widehat{\mathcal{T}} = \int d\omega_1 \cdots d\omega_n \delta(\omega_1 - \omega).$$

(12)

The function

$$P_h(\omega) = \widehat{\mathcal{T}} \exp(-\beta h),$$

(13)

(with the parameters $\sigma_{\alpha\beta}$ determined by the stationarity conditions which were discussed above) constitutes an approximation to the exact spatial probability distribution, averaged over the random realizations of the potential, and given by the formula

$$P_H(\omega) = \left(\frac{\exp(-\beta H(\omega))}{\int d\sigma \exp(-\beta H(\sigma))}\right) = \widehat{\mathcal{T}} \exp(-\beta H),$$

(14)

with the limit $n \to 0$ to be understood. Equation (13) has been evaluated by us in a previous publication [16] and compared with numerical simulations both using the RS and RSB solutions for the variational parameters. The result for $P_h$ is [16]:

$$P_h(\omega) = \left(\frac{\beta}{2\pi G_{11}}\right)^{1/2} \exp(-\frac{\beta \omega^2}{2G_{11}}),$$

(15)

with

$$G_{ab} = \left[\mu I - \hat{\sigma}\right]^{-1}_{ab}.$$

(16)

Substituting the RS and RSB solutions for $G_{11}$ obtained in reference [13], we find [16]

$$P_h(\omega) = \left(\frac{\beta \mu}{2\pi(1 + \gamma^{-1}\hat{T}^{-1}(1 + \gamma))}\right)^{1/2} \exp\left(-\frac{\beta \mu \omega^2}{2(1 + \gamma^{-1}\hat{T}^{-1}(1 + \gamma))}\right), \quad \hat{T} > 1$$

$$P_h(\omega) = \left(\frac{\beta \mu \gamma \hat{T}}{2\pi(1 + \gamma)}\right)^{1/2} \exp\left(-\frac{\beta \mu \gamma \hat{T}}{2(1 + \gamma)} \omega^2\right), \quad \hat{T} < 1$$

(17)

with the 'reduced' temperature $\hat{T}$ defined as

$$\hat{T} = \beta^{-1}\mu^{\frac{1}{2\gamma}} \left(\gamma^{2^{1-2\gamma}} \frac{\Gamma(3/2 - \gamma)}{\Gamma(1/2)} g\right)^{-\frac{1}{1+\gamma}}$$

(18)

In the sequel we refer to the expressions given in equation (17) as "the Hamiltonian variational approximation".

I proceed to derive a new variational scheme which is more appropriate for approximating the position-dependent spatial probability distribution. The idea is to use the inequality (6), but substitute $\widehat{\mathcal{T}}$ from equation (12) for the trace in equation (8). This means, defining

$$\langle \langle A \rangle \rangle(\omega) \equiv \frac{\widehat{\mathcal{T}} \left[A(\omega_1, \cdots, \omega_n) \exp(-\beta h)\right]}{\widehat{\mathcal{T}} \exp(-\beta h)}$$

(19)
The notation \( \langle \rangle \) is used to distinguish the \( \omega \)-dependent average from the averaged defined in equation (8). Using \( A = -\beta (H - h) \) I find

\[
P_H(\omega) = \operatorname{Tr} \exp (-\beta H) \geq \exp (-\beta \langle (H - h) \rangle (\omega)) \times \operatorname{Tr} \exp (-\beta h) \equiv P_v(\omega) \quad (20)
\]

Again, for positive integers \( n \), and \( \operatorname{Tr} \exp (-\beta h) < \infty \), the measure

\[
\left[ \operatorname{Tr} \exp (-\beta h) \right]^{-1} \exp (-\beta h) \delta(\omega_1 - \omega) \, d\omega_1 \cdots d\omega_n ,
\]

is a positive measure on \( \mathbb{R}^n \) for any value of \( \omega \) and the inequality (6) holds. For \( n \to 0 \) this is no longer true, but the stationary point of the r.h.s. of equation (20), denoted by \( P_v(\omega) \), with respect to the parameters \( \sigma_{ab} \) is expected to yield a good approximation to the spatial probability distribution by virtue of analytic continuation. This will be checked in section 4 in comparison with numerical simulations. Such a variational determination of \( P_v(\omega) \) is obtained for each value of \( \omega \) separately and thus it is expected to provide a better approximation than by just using the \( \sigma_{ab} \) obtained globally from extremizing the free energy (see Eq. (10)), and using equation (13). One should note that it does not follow from our discussion that \( P_v(\omega) \) is properly normalized. Provided it is a good approximation to the exact probability distribution, its normalization will be close to one, and correcting for the exact normalization will have practically no effect on the behavior in the tail region were the probability is very small and where the variational calculation is most important.

Our next task is to evaluate the quantity \( \langle (H - h) \rangle (\omega) \) needed in order to calculate \( P_v(\omega) \), see equation (20). If we use the integral representation for the Dirac \( \delta \)-function in equation (12):

\[
\delta(\omega_1 - \omega) = \int \frac{dk}{2\pi} e^{ik\omega_1 - ik\omega}
\]

we can write

\[
\operatorname{Tr} [ (H - h) \, e^{-\beta h} ] = \int \frac{dk}{2\pi} e^{ik\omega} \int d\omega_1 \cdots d\omega_n \\
\times \left( \frac{\beta}{2} \sum_{ab} f((\omega_a - \omega_b)^2) + \frac{1}{2} \sum_{ab} \sigma_{ab} \omega_a \omega_b \right) \times \exp \left( -\frac{\beta}{2} \sum_{ab} (G^{-1})_{ab} \omega_a \omega_b - ik\omega_1 \right) .
\]

In the Appendix we show how the integrals can be evaluated for general \( n \). The end result is:

\[
\langle (H - h) \rangle (\omega) =
\]

\[
= \frac{\beta}{2} \left( \frac{G_{11}}{\pi} \right)^{1/2} \exp \left( \frac{\beta \omega^2}{2G_{11}} \right) \sum_{ab} (Z_{ab})^{-1/2} \int_{-\infty}^{\infty} dp \, \exp \left( -p^2 - \frac{(\omega \sqrt{\beta} + p \sqrt{2} Y_{ab})^2}{2Z_{ab}} \right)
\]

\[
\times f \left( \frac{2}{\beta} X_{ab} p^2 \right) - \frac{n}{2\beta} + \frac{\mu}{2\beta} \sum_a G_{aa} + \frac{1}{2\beta G_{11}} (G_{11} - \mu) \sum_a G_{1a}^2 (1 - \frac{\beta \omega^2}{G_{11}})
\]

with

\[
X_{ab} = G_{aa} + G_{bb} - 2G_{ab}
\]

\[
Y_{ab} = (G_{1a} - G_{1b}) / (X_{ab})^{1/2}
\]

\[
Z_{ab} = G_{11} - Y_{ab}^2
\]

(25)
For the special case of interest $\gamma = 1/2$ (see Eq. (2) for $f$) we find:

$$
\langle (H - h) \rangle (\omega) = \sum_{a} \left[ \frac{\beta Y_{ab} X_{ab}^{1/2}}{2 G_{11}} \right. \\
- \frac{n}{2 \beta} + \frac{\mu}{2 \beta} \sum_{a} G_{aa} + \frac{1}{2 \beta G_{11}} (G_{11} - \mu \sum_{a} G_{11}^{2}) (1 - \beta \omega^{2}/G_{11}),
$$

(26)

where erf is the usual error function. Equations (24) and (26) together with the expression (20) for $P_{\nu}(\omega)$ constitute the main results of this section. In the rest of the paper we consider only the important case of $\gamma = 1/2$.

3. The replica symmetric solution.

In this section we consider the replica symmetric solution to the variational stationarity equations. In this case we search for a solution for which all the off diagonal elements of the matrix $\sigma_{ab}$ are equal as well as all the diagonal elements:

$$
\sigma_{ab} = \sigma \quad a \neq b \\
\sigma_{aa} = \sigma_{d} \quad a = 1 \cdot n
$$

(27)

we also define

$$
\mu_{1} = \mu + \sigma_{d} + (n - 1) \sigma
$$

(28)

In terms of these parameters one finds

$$
G_{aa} = \frac{1}{\mu_{1}} \left( 1 + \frac{\sigma}{\mu_{1}} \right) ; \quad G_{ab} = \frac{\sigma}{\mu_{1}^{2}}, \quad a \neq b
$$

(29)

Thus we have two variational parameters $\sigma$ and $\mu_{1}$ as contrasted with the Hamiltonian variational approach were there is only one variable because in that case translational invariance dictates $\mu_{1} = \mu$. In addition, the variational parameters are of course dependent on $\omega$ in the present case. We define for convenience:

$$
\Gamma = G_{11} + G_{12}.
$$

(30)

Using the result of the previous section, equation (26), we can express the probability distribution $P_{\nu}(\omega)$ (see also Eqs.(20) and (13)) as

$$
P_{\nu}(\omega) = \left( \frac{\beta}{2 \pi G_{11}} \right)^{1/2} \exp \left( -\frac{\beta \omega^{2}}{2 G_{11}} \right) \exp \left( g(\omega) \right)
$$

$$
g(\omega) = \frac{g \beta^{2} \omega}{\mu_{1} G_{11}} \exp \left( \frac{\beta}{2 \mu_{1} G_{11}} \right)^{1/2} \omega + g \beta \left( \frac{2 \beta \Gamma}{\pi \mu_{1} G_{11}} \right)^{1/2} \exp \left( -\frac{\beta \omega^{2}}{2 \mu_{1} \Gamma G_{11}} \right)
$$

$$
-2 g \beta \left( \frac{\beta}{\pi \mu_{1}} \right)^{1/2} - \frac{1}{2} \left( 1 - \frac{\mu \Gamma}{\mu_{1} G_{11}} \right) \left( 1 - \frac{\beta \omega^{2}}{G_{11}} \right),
$$

(31)

where the limit $n \to 0$ has been taken. The stationary points of equation (31) in the $\sigma - \mu_{1}$ plane as functions of $\omega$, have been obtained numerically for various values of the parameters...
of the model \( (\beta, \mu, g) \), and the results have been used back in equation (31) to evaluate \( P_\nu(\omega) \).

The results will be summarized below. But first let us examine the simpler behavior in the tail of the probability distribution, that can be investigated analytically.

For large values of \( \omega \), the error-function in equation (31) can be approximated by \( \text{sign}(\omega) \) and the exponential term in the expression for \( g(\omega) \) is negligible. If we further define the tail region as the region for which

\[
|\omega| >> \beta g / \mu ,
\]

we find that the extremum of \( P_\nu(\omega) \) is obtained for

\[
\frac{\sigma}{\mu_1} \approx \frac{\beta g}{\mu|\omega| - \beta g} ,
\]

\[
\mu_1 \approx [\mu\pi + 2\beta^3 g^2 - 2g\beta(\beta^4 g^2 + \beta\mu\pi)^{1/2}] / \pi .
\]

Plugging these expressions back into the expression for \( P_\nu(\omega) \) one finds that the behavior of the spatial probability distribution in the tail region defined by equation (32) is

\[
P_\nu(\omega) \approx \exp(-\mu\beta \omega^2 / 2 + g\beta^2 |\omega| + C)
\]

\[
C = -\frac{\beta^3 g^2}{2\mu} - 2\beta g \left( \frac{\beta}{\pi\mu_1} \right)^{1/2} + \frac{\mu}{2\mu_1} - \frac{1}{2} + \frac{1}{2} \ln \left( \frac{\beta\mu_1}{2\pi} \right) ,
\]

where \( \mu_1 \) is given by equation (33).

The extremum in the tail turns out to be a minimum in the \( \sigma - \mu_1 \) plane, as opposed to the situation for \( n \geq 1 \) when it is a maximum as can be seen from equation (20). (On the contrary, for very small values of \( \omega \) we have found numerically, that the stationarity point is actually a saddle point.) The fact that the extremum in the tail region is a minimum seems to suggest that the approximate expression equation (34) constitutes an upper bound to the exact behavior. The behavior in the tail given by equation (34) should be compared with the behavior obtained from the conventional variational approximation given by substituting \( \gamma = 1/2 \) in equation (17). Those formulas give a higher value for the tail than that predicted by equation (34). (This is true even when \( T < 1 \) with the RSB solution). More on this in the discussion below.

4. Comparison with numerical simulations.

We proceed to a numerical comparison between simulations and the results of the various variational approximations. Again, we limit the discussion to the case \( \gamma = 1/2 \). We have studied numerically a lattice version of the toy model. A suitable interval of the particle's position \( \omega \ ( -12.5/\sqrt{\beta} < \omega < 12.5/\sqrt{\beta} \) ) is divided into 5,000 lattice sites. For a given realization, the algorithm generates an independently distributed Gaussian random number for each site \( r_i \); it then generates \( V_j \), the correlated random potential at site \( j \), by summing the random numbers in the following way:

\[
V_j \propto \sum_i \text{sign}(i - j) r_i .
\]

The quadratic term of the Hamiltonian is added to this random potential, and then the partition function and probability distribution are calculated.

We consider three sets of values for the parameters \( (\beta, g, \mu) : (0.2, 2\sqrt{\pi}, 1), (1.0, 2\sqrt{\pi}, 1), (10.0, 2.2, 4.6) \). The corresponding values of the reduced temperature \( T \) for these three cases
Fig. 1. — Plot of the log of spatial probability distribution vs. $\omega^2$ for $\hat{T} = 5$ (solid line). The dashed line is the result of the Hamiltonian variational approximation and the diamonds the results of our new variational scheme.

are 5, 1 and 0.23 respectively. The data for $\hat{T} = 5$ is plotted in figure 1 (solid curve). It was obtained from numerical simulations with 50000 realizations of the disorder. The dashed line represents the probability $P_h$ given in equation (17) and derived from the Hamiltonian variational method. The diamonds represent the approximation developed in the last section. We see that it gives a perfect fit to the data for this value of $\hat{T}$. We have used Mathematica to find the stationary point of equation (31) in the $\mu_1 - \sigma$ plane and then substituted these values back into equation (31). The asymptotic formula equation (34) predicts

$$P_v(\omega) \approx \exp(-0.1\omega^2 + 0.142\omega - 2.1)$$

where we used $\mu_1 = 0.7$ from equation (33). This behavior is also indistinguishable from the data in the range $10 < \omega < 28$.

Let us proceed to the case $\hat{T} = 1$. The data is plotted in figure 2. In this case the noise associated with the random potential is apparent. In this case we found it necessary to average over 500000 realizations. The data for 50000 realizations is also shown in lighter dots. In the tail region it is apparent that the curve corresponding to the lower number of realizations has a lower value, since the average is increased by relatively rare events. The dashed curve is the single parameter Hamiltonian variational fit. The new variational method results are represented by the diamonds. The asymptotic formulas predicts $\mu_1 = 0.06$ and

$$P_v(\omega) \approx \exp(-0.5\omega^2 + 3.545\omega - 17).$$

It is represented by the solid line in the figure. The diamonds do not lie exactly on this line, because $\omega$ is still not large enough in this range. Again we see that the variational approximation gives an excellent fit to the data.

The final example is for $\hat{T} = 0.23$ using $10^6$ realizations of the disorder. The data is depicted in figure 3. The dashed line is the result of the Hamiltonian RS variation. The dot-dashed line
Fig. 2. — Plot of the log of the spatial probability distribution vs. $\omega^2$ for $\hat{T} = 1$. The wiggly solid curve represent the result of averaging over 500000 realizations. The light wiggly curve is for 50000 realizations. The dashed curve and the diamonds are explained in the caption of figure 1. The solid smooth curve result from the asymptotic formula, equation (34).

is the result of the RSB Hamiltonian variation which is the appropriate solution for $\hat{T} < 1$. The diamonds again represent our new variational method results. The range of $\omega$ simulated is lower than the onset of the tail region given by equation (32) which in the present case starts above $\omega \sim 5$, so a comparison with the asymptotic formula equation (34) is not shown.

We see that the data in this case falls below the result of our variational method, which is nonetheless better than the Hamiltonian RSB variational approximation. Two possibilities come to mind to explain this discrepancy.

1. It seems quite possible that because the relative strength of the random part of the potential is much larger when $\hat{T}$ is small, as compared to the harmonic part, one needs more realizations to accumulate enough statistics for the averaged probability distribution. For $\hat{T} = 5$ even 5000 realizations already gave us good results. In figure 1 we show the results for 50000 realizations, but these are practically indistinguishable from the average of 5000 realizations. For $\hat{T} = 1$, 50000 realizations are not sufficient and we had to average at least 500000 realizations to accumulate enough statistics. This is because we have to collect enough rare events which contribute to the distinction between the average and typical values of the spatial probability distribution [15, 16]. It is quite plausible that to get better results for $\hat{T} = 0.23$ one has to go to a higher number of realizations. Averaging over more realizations (see e.g Fig. 2 for the distinction between 50000 and 500000 realizations) may narrow the gap between the data and the variational approximation.

2. Another strong possibility is that like the Hamiltonian variational case it is necessary for small $\hat{T}$ to look for a solution with replica symmetry breaking when using the current variational scheme. Such a solution may display a different asymptotic behavior for small $\hat{T}$ than the one given by equation (34). It may also yield a lower value in the pretail region (which is the range of values depicted in Fig. 3). In order to find such a solution one has to go back to
Fig. 3. — Plot of the log of the spatial probability distribution vs. $\omega^2$ for $\hat{T} = 0.23$. The wiggly solid curve represents the result of averaging over $10^6$ realizations. The dashed and dashed-dotted lines represent the Hamiltonian RS and RSB approximations respectively. The diamonds are the results of the new variational scheme. The open triangles represent the empirical cubic approximation.

the full expressions derived in section 2 without making the simplifying assumptions of replica symmetry made in section 3, and one has to extremize the probability distributions under the more general conditions. The task of finding a RSB solution is left for future research.

5. Discussion.

In this paper we have developed a new variational scheme for approximating the spatial probability distribution. The replica symmetric solution gives an excellent approximation to the numerical data for high temperatures $\hat{T} > 1$. For the tail of the spatial probability it predicts a Gaussian decay with a linear exponential correction. At lower temperature, the fit in the tail region is not that good, either because the numerical data is insufficient and one needs to average over a higher number of realizations, or a solution with replica symmetry breaking is needed (or both). Of course since we are dealing after all with an approximation, we are never guaranteed a perfect fit. For all temperatures tested the present method gives a much better fit to the probability distribution than using the Hamiltonian variational method, both with or without RSB.

When the data for $\hat{T} = 0.23$ is displayed in a log-log plot, [16] a crossover is observed from a behavior $P \sim \exp(-\text{const} \omega^2)$ to a behavior like $P \sim \exp(-\text{const} \omega^3)$. An empirical fit to the data of the form

$$P(\omega) \sim \exp(-3.5\omega^3 + 20)$$

(38)

is depicted as open triangles in figure 3 for the range $6 < \omega^2 < 16$. Since in this case we are not really observing the tail region (according to the definition given in Eq. (32)), this behavior
may be a transient or intermediate behavior. We should also be cautious about the data in
this region, because as mentioned in the last section it is possible that more realizations are
needed.

On the other hand, if we do take the cubic $\omega$ dependence of the log of the probability
distribution seriously, this immediately rings a bell because of some work done by Villain et al.
[1] on the toy model. What they actually showed was that the probability for rare realizations
of the disorder which make $H(\omega) \sim 0$ and thus $\exp(-\beta H) \sim 1$ behaves like
$\sim \exp(-\omega^3 \mu^2 / 2g)$, for values of $\omega^3 \gg 2g/\mu^2$ (I have transformed their notation to ours). This could lead to
the conclusion that the spatial probability distribution should also behave like a cubic power
of $\omega$. This is true only if the probability distribution is completely dominated by the rare
realizations of this kind, a fact that was never claimed by Villain et al. It is certainly possible
that other realizations which give lower values to $\exp(-\beta H)$ but are nonetheless more abundant
dominate the average value. Villain’s argument is valid for any temperature. Our numerical
results show that one certainly does not get a cubic behavior of the probability distribution
at high temperature for values of $\omega \gg (g/\mu^2)^{1/3}$. In that case the rare realizations of of the
type considered by Villain still exist but they do not dominate the probability distribution.

This is actually easy to understand. Let us define two different length scales in the problem.
The first, introduced by Villain et al. which we call $\xi_1$ is defined as

$$\xi_1 \simeq \left( \frac{2g}{\mu^2} \right)^{1/3}.$$  \hfill (39)

is the length above which the probability for rare events of magnitude 1 goes like

$$A \exp\left(-\frac{\omega^3}{\xi_1^3}\right)$$  \hfill (40)

with some undetermined constant $A$. The second length, which I introduced in equation (32),

$$\xi_2 \simeq \frac{\beta g}{\mu},$$  \hfill (41)

is the length for which the asymptotic behavior in the tail starts according to our investigation
in section 3. For $\omega$ above this value we have found the behavior

$$P(\omega) \simeq \exp(-\beta\mu\omega^2 / 2 + g\beta^2 |\omega| + C(\beta)),$$  \hfill (42)

where $C(\beta)$ is given in equation (34). Since

$$\xi_2 \simeq \xi_1 \times \frac{(2\pi)^{1/3}}{T}$$  \hfill (43)

We see that for $T > 1.8$, the cubic behavior is never realized since the contribution of the rare
realizations of the Villain type to the averaged probability is smaller than the behavior given
by equation (42). This explain the perfect fit of the asymptotic behavior given in equation
(37) and the numerical data, starting at a very low value of $\omega$.

On the other hand for $T << 1.8$ it is conceivable to have two tail regimes, the first with
$\xi_1 < \omega < \xi_2$ in which the probability has the cubic behavior in $\omega$ because it is dominated
by rare configurations of the Villain type, and a second tail regime for $\omega > \xi_2$ for which the
asymptotic behavior is changed to a quadratic behavior given by equation (42), if the results
of the RS solution are valid (or possibly to a different asymptotic behavior which will emerge
from a RSB solution). This is because one can easily check that at the border between these
two regimes the two expressions given by equation (40) and equation (42) become comparable
in magnitude, and the quadratic behavior wins for \( \omega > \xi_2 \). As the (reduced) temperature is
lowered from 1 the first regime (cubic behavior) is expected to grow in size and include all of
the tail at \( T = 0 \). Simulations of directed polymers at zero temperature, which can be mapped
into corresponding results for the toy-model \([9] \), showed the beginning of a change in the form
of the spatial probability distribution from \( \sim \exp(-\omega^2) \) to \( \sim \exp(-\omega^{2.2}) \) at the onset
of the tail, but did not go far enough into the tail region to confirm a cubic dependence. See
also reference \([14] \). We have previously observed cubic dependence in the tail of the directed
polymers' spatial probability distribution at finite temperature \([15] \).

There is some difficulty though, to explain the apparent cubic behavior in figure 3 purely in
terms of Villain's configurations because we simulated "only" over \( 10^6 \) realizations and thus
if the average is dominated by a single realization whose contribution is unity, the value of
the average should be of the order of \( 10^{-6} \approx \exp(-14) \) which far exceeds the value of the
distribution in most of this region (except at the very beginning). One might argue that there
are other realizations with somewhat smaller contributions to the average than Villain's which
also gives rise to a similar cubic behavior but this needs to be verified.

We hope that this work will stimulate further investigation of the behavior of the tail of the
probability distribution at low temperatures. Three important questions that need a definite
answer are

1. Is there a RSB solution to our new variational equations?
2. Is a cubic dependence of the log of the probability indeed realized over a large region when
   the temperature is very low?
3. Is the asymptotic behavior given by equation (34) which works so well for high temperatures
   when \( \omega > \xi_2 \), also valid asymptotically at low temperatures?

We also hope that it will be possible to extend the variational method developed in this
paper for the zero-dimensional manifold directly to higher dimensional manifolds in random
media.

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Appendix A.

In this Appendix we derive equation (24) starting from equation (23). Let us shift the variables
\( \omega_a \) in equation (23)

\[
\omega_a \to \omega_a + \lambda_a
\]

(A.1)
such that the linear term in \( \omega_1 \) in the exponential is eliminated. This is achieved by choosing

\[
\lambda_a = -(i/\beta)G_{1a}k
\]

(A.2)
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We then find:

\[
\overline{\operatorname{Tr}} \left[ (\mathcal{H} - h) e^{-\beta h} \right] = \int \frac{dk}{2\pi} e^{ik\omega} e^{-\beta \frac{G_{11} k^2}{2}} \int d\omega_1 \cdot d\omega_n \times \left( \frac{\beta}{2} \sum_{ab} f((\omega_a - \omega_b + \lambda_a - \lambda_b)^2) + \frac{1}{2} \sum_{ab} \sigma_{ab}(\omega_a + \lambda_a)(\omega_b + \lambda_b) \right) \times \exp \left( -\frac{\beta}{2} \sum_{ab} (G^{-1})_{ab} \omega_a \omega_b \right).
\]

(A.3)

We now expand the function \( f \) in a power series about 0, (this is used only as a tool derive our result. It may not be necessary for \( f \) to be analytic about 0)

\[
f(x) = \sum_{l=0}^{\infty} f_l x^l
\]

(A.4)

We use the following formula to integrate over \( \omega_1 \cdots \omega_n \):

\[
\int d\omega_1 \cdot d\omega_n \left( \omega_a - \omega_b \right)^{2s} \exp \left( -\frac{\beta}{2} \sum_{ab} (G^{-1})_{ab} \omega_a \omega_b \right) = (2\pi/\beta)^{n/2} (\det G)^{1/2} \frac{2\Gamma(1/2 + s)}{\beta^s \Gamma(1/2)} (G_{aa} + G_{bb} - 2G_{ab})^s,
\]

provided \( s \) is a non-negative integer. For \( s \) being half-integer the integral is 0. We obtain

\[
\overline{\operatorname{Tr}} \left[ (\mathcal{H} - h) e^{-\beta h} \right] = \left( \frac{G_{11}}{2\pi \beta} \right)^{1/2} e^{-\beta \frac{G_{11} k^2}{2\pi}} \int dk \left\{ \exp \left( ik\omega - \frac{1}{2\beta} G_{11} k^2 \right) \times \frac{\beta}{2} \sum_{ab} \hat{f} \left( -(G_{1a} - G_{1b})^2 k^2 / \beta^2, (G_{aa} + G_{bb} - 2G_{ab}) / \beta \right) \exp \left( -\frac{\beta}{2} \sum_{cd} (G^{-1})_{cd} \omega_a \omega_d \right) \right\}
\]

\[
- \frac{n}{2\beta} + \frac{\mu}{2\beta} \sum_a G_{aa} + \frac{1}{2\beta G_{11}} \left( G_{11} - \mu \sum_a G_{1a}^2 \right) \left( 1 - \beta \omega^2 / G_{11} \right)
\]

(A.6)

where

\[
\hat{f}(x, y) = \frac{1}{\sqrt{\pi}} \sum_{l=0}^{\infty} f_l \left( 2y \right)^l \sum_{s=0}^{l} g(l, s) \Gamma(s + 1/2) \left( \frac{x}{2y} \right)^{l-s}
\]

\[
g(l, s) = \sum_{j=0}^{l} \sum_{m=0}^{\infty} \delta_{(j+m)/2, s} \binom{l}{j} \binom{j}{m} 2^{-m}
\]

(A.7)

Since

\[
\int_{-\infty}^{\infty} dp e^{-p^2} (p + q)^{2l} = \sum_{s=0}^{l} g(l, s) \Gamma(s + 1/2) q^{2(l-s)},
\]

we see that \( \hat{f}(x, y) \) can be expressed in the form

\[
\hat{f}(x, y) = \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} dp e^{-p^2} f \left( 2y \left( p + \sqrt{\frac{x}{2y}} \right)^2 \right) = e^{-\frac{x}{2y}} \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} dp f(2yp) e^{-p^2 + 2\sqrt{z/(2y)} p}
\]

(A.9)
Using this representation for \( \tilde{f}(x,y) \) the integral over \( k \) in equation (A.6) can be performed, and we obtain the desired result given in equation (24).

References