Thermal Equilibrium with the Wiener Potential: Testing the Replica Variational Approximation

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Abstract. – We consider the statistical mechanics of a classical particle in a one-dimensional box subjected to a random potential which constitutes a Wiener process on the coordinate axis. The distribution of the free energy and all correlation functions of the Gibbs states may be calculated exactly as a function of the box length and temperature. This allows for a detailed test of results obtained by the replica variational approximation scheme. We show that this scheme provides a reasonable estimate of the averaged free energy. Furthermore our results shed more light on the validity of the concept of approximate ultrametricity which is a central assumption of the replica variational method.

The replica trick and Parisi’s scheme of replica symmetry breaking within mean field theories provided a promising step towards the application of powerful methods of field theory to systems with quenched random couplings [1]. More recently these concepts have been applied to a variety of physical systems as an approximation scheme within a framework called “replica variational approximation” (RVA). The strategy of the RVA [2] is to calculate variational bounds on the moments of the canonical partition sum within an ensemble of quenched disordered couplings. For integer $n > 0$ these bounds can be achieved from standard inequalities of equilibrium statistical mechanics. Disorder averaged physical quantities are estimated from these bounds by using the “$n \to 0$” trick $\ln(x) = \lim_{n \to 0} (x^n - 1)/n$. The method has been tested using toy models of manifolds in random media [3, 4]. In the limit of a manifold embedded in infinite dimensional space the RVA with a Gaussian trial distribution becomes exact. For a zero dimensional manifold in one dimensional space the test has used exact results on certain linear combinations of moments of the manifold’s position which have been obtained some time ago [5]. In a more recent work [6] the probability distribution of the free energy of a related model defined on the half axis has also been obtained.

The purpose of the present letter is twofold. First, we give a complete solution of the zero dimensional toy model. We use the expression “complete” to indicate that
the solution does not only provide an explicit analytical expression for the probability density of the free energy for arbitrary temperatures and system sizes but also allows us to calculate all correlation functions of the Gibbs state (canonical distribution). In this way we completely characterize the probability functional of the Gibbs state which contains all the statistical information on the thermostatistics of the disordered system. Second we use our results to test the quality of the RVA.

We consider the position \( x \) of a classical particle in a one-dimensional box \( 0 \leq x \leq L \) subjected to a random potential. On the one hand we will use for the random potential the standard Wiener process \( W(x) \), that is, the Gaussian Markov process with averages \( \langle W(x) \rangle = 0 \) and \( \langle W(x)W(y) \rangle = \min(x,y) \). But mainly we will focus our interest on its variant \( V(x) := W(x) - W(L)/2 \). Below we will refer to these potentials as the \( W \)- and \( V \)-ensemble, respectively. A single particle moving under the influence of the potential \( V(x) \) may be considered as a continuum model of a kink in an Ising chain with random fields uncorrelated at different sites \([7]\) whereas the \( W \)-ensemble is related to the asymptotic behaviour of a directed polymer in a random potential in \( 1+1 \) dimensions \([8]\). Note that the Gaussian random potential \( V(x) \) is equivalently characterized by the translationally invariant averages \( \langle V(x) \rangle = 0 \) and \( \langle V(x)V(y) \rangle = (L/2 - |x-y|)/2 \). The position \( x \) of a particle in contact with a heat bath of fixed inverse temperature \( \beta \) is distributed according to the Gibbs state \( \Omega_{\beta,L}(x) := \exp\{ -\beta V(x)/Z_{\beta}(L) \}/Z_{\beta}(L) \). In the following we will be interested in statistical properties of this state, the corresponding partition sum \( Z_{\beta}(L) := \int_0^L dx \exp\{ -\beta V(x) \} \) and the free energy \( F_{\beta}(L) := -\beta^{-1} \ln Z_{\beta}(L) \) within the \( V \)-ensemble. Our general strategy will be to calculate such properties from corresponding properties of the \( W \)-ensemble with partition sum \( \tilde{Z}_{\beta}(L) := \int_0^L dx \exp\{ -\beta W(x) \} \) and free energy \( \tilde{F}_{\beta}(L) := -\beta^{-1} \ln \tilde{Z}_{\beta}(L) \).

Throughout our calculations we find it convenient to use scaled variables for locations, potentials and partition sums defined as: \( s := \beta^2 x/8 \), \( v(s) := -(\beta/2)V(8s/\beta^2) \), \( w(s) := -(\beta/2)W(8s/\beta^2) \), \( z(s) := (\beta^2/2)Z_{\beta}(8s/\beta^2) \), and \( \tilde{z}(s) := (\beta^2/2)\tilde{Z}_{\beta}(8s/\beta^2) \). The scaled system length will be denoted by \( l := \beta^2 L/8 \). The transition density \( p_s(w,\tilde{z}|w_0,\tilde{z}_0) \) of the homogeneous Markov process \((w(s),\tilde{z}(s))\) may be determined from the Fokker-Planck equation

\[
\partial_s p_s(w,\tilde{z}|w_0,\tilde{z}_0) = \left( \partial_w^2 - 4e^{2w} \partial_{\tilde{z}} \right) p_s(w,\tilde{z}|w_0,\tilde{z}_0) \tag{1}
\]

with initial condition \( p_0(w,\tilde{z}|w_0,\tilde{z}_0) = \delta(w-w_0)\delta(z-z_0) \). This equation is equivalent to the Langevin equations \( dw(s)/ds = \sqrt{2} \xi(s) \) and \( d\tilde{z}(s)/ds = 4e^{2w(s)} \) following immediately from the definitions of \( w(s) \) and \( \tilde{z}(s) \). Here \( \xi \) denotes standard Gaussian white noise with \( \langle \xi(s) \rangle = 0 \) and \( \langle \xi(s)\xi(s') \rangle = \delta(s-s') \). To obtain the joint probability density of \( v(s) \) and \( z(s) \) from the transition density of \( w(s) \) and \( \tilde{z}(s) \) we use the relation

\[
\begin{align*}
\left\langle \delta(z(s) - z)\delta(v(s) - v) \right\rangle &= \int_{-\infty}^{\infty} dw e^{\nu} \int_{-\infty}^{\infty} d\tilde{z} \ p_l(w,\tilde{z}|v + \frac{1}{2} w, e^{\nu} z) \ p_s\left(w + \frac{1}{2} w, e^{\nu} z \big| 0, 0 \right) .
\end{align*}
\tag{2}
\]

Note that according to \([11]\) one has

\[
p_s(w,\tilde{z}|w_0,\tilde{z}_0) = p_s(w,\tilde{z} - \tilde{z}_0|w_0,0) . \tag{3}
\]

To solve the Fokker-Planck equation \([11]\) we perform a Laplace transform with respect to \( \tilde{z} \) and introduce

\[
\tilde{p}_s(w,\varrho|w_0) := \int_0^{\infty} d\tilde{z} e^{\varrho \tilde{z}} p_s(w,\tilde{z}|w_0,0) . \tag{4}
\]
which obeys the equation

$$\left( \partial_s - \partial_w^2 + 4\varrho e^{2w} \right) \tilde{p}_s(w, \varrho|w_0) = 0$$  \hspace{1cm} (5)$$

with initial condition $\tilde{p}_0(w, \varrho|w_0) = \delta(w - w_0)$. Thus we see that $\tilde{p}$ becomes a Green function of a Bessel-type differential equation. It may be given in terms of an eigenfunction expansion

$$\tilde{p}_s(w, \varrho|w_0) = \frac{2}{\pi^2} \int_0^\infty d\nu \nu \sinh(\pi\nu) e^{-\nu^2 s} K_{i\nu}(2\sqrt{\varrho} e^w) K_{i\nu}(2\sqrt{\varrho} e^{w_0}),$$  \hspace{1cm} (6)$$

where $K_{i\nu}(y) = \int_0^\infty dt \cos(t\nu) \exp\{-y \cosh t\}$ denotes the modified Bessel function of third kind with index $i\nu$, see [9, Chap. 9]. As to the validity of (6) we remark that $e^{-\nu^2 s} K_{i\nu}(2\sqrt{\varrho} e^w)$ obeys (6) for all $\nu$ which can be checked with the help of the differential equation [9, Eq. 9.6.1] for the modified Bessel functions. Furthermore, the right-hand side of (6) reproduces the demanded initial condition which can be inferred from the pair [10, p. 173] of reciprocal formulas for the Kontorovich-Lebedev transformation.

In the sequel we will summarize some of our results on the statistics of the free energy and the Gibbs state. All of these results can be obtained from the fundamental solution (6). A detailed exposition of the calculations and the results will be given in [11].

For the discussion of the statistical properties of the free energies it is convenient to introduce their scaled variants $f(l) := -l^{-1/2} \ln(z(l))$ and $\hat{f}(l) := -l^{-1/2} \ln(\hat{z}(l))$ from which the original quantities can be recovered according to

$$F_\beta(L) = \frac{1}{2} \sqrt{\frac{L}{2}} f\left(\frac{\beta^2}{8} L\right) + \frac{1}{\beta} \ln \frac{\beta^2}{2}$$  \hspace{1cm} (7)$$

and analogously for $\hat{F}_\beta(L)$. As $z(l) = e^{-w(l)} \hat{z}(l)$, the averaged free energy is the same for both ensembles, that is, $\langle f(l) \rangle = \langle \hat{f}(l) \rangle$. Fluctuations of the free energy, however, will differ between the two ensembles. For example, one has $\langle (f(l))^2 \rangle = \langle (\hat{f}(l))^2 \rangle - 2$ as shown in [11].

The density of the free energy $f(l)$ turns out to be

$$\langle \delta(f(l) - f) \rangle = \frac{2}{\pi \sqrt{\pi}} \exp\left\{ \frac{\pi^2}{4l} + f\sqrt{l} \right\} K_0\left(2e^{f\sqrt{l}}\right) \times \int_0^\infty dt \sinh(t) \sin\left(\frac{\pi}{2l} t\right) \exp\left\{-\frac{l^2}{4l} - 2e^{f\sqrt{l}} \cosh(t)\right\}.$$  \hspace{1cm} (8)$$

In Fig. [4] a plot of the centered density of $f(l)$ is given for different values of $l$. An expression analogous to (8) for the density of $\hat{f}(l)$ will be given in [11].

Of course, the densities allow for a calculation of the averaged free energies and their fluctuations. Here we only give the asymptotic expansion of the averaged free energy for $l \to \infty$

$$\langle f(l) \rangle = \langle \hat{f}(l) \rangle = -\frac{4}{\sqrt{\pi}} - \frac{\gamma}{\sqrt{l}} + \frac{\pi \sqrt{\pi}}{6l} + O(l^{-2}),$$  \hspace{1cm} (9)$$

where $\gamma = 0.5772\ldots$ denotes the Euler-Mascheroni constant [3, Eq. 6.1.3].

In order to get along with the calculation of the averaged free energy within the RVA using the standard Gaussian trial distributions we extend the system to the whole real axis by softening the walls. More precisely, we use the potential $v(s) + (1 - 2s/l)^{2M}$, $s
real, $M = 1, 2, 3, \ldots$, instead of $v(s)$ for the calculations and eventually perform the limit $M \to \infty$. For this setting we have re-done the RVA along the lines of [2]. The details will be given in [11]. The results of the RVA to the averaged free energy $\langle f(l) \rangle \approx f^{\text{RVA}}(l)$ are as follows. For $l < \sqrt{3\pi}$ the saddle-point equations have a replica symmetric solution only, resulting in

$$f^{\text{RVA}}(l) := f^{\text{RS}}(l) := -\frac{1 + \sqrt{2}}{\sqrt{\pi}} \nu_l \sqrt{l} - \frac{1}{2\sqrt{l}} \left(1 + \ln\left(8\pi l^2 \nu_l^2\right)\right), \quad \text{for } l < \sqrt{3\pi},$$

(10)

where $0 \leq \nu_l \leq 1$ solves $\frac{2l}{\sqrt{\pi}} \nu_l^2 + \nu_l^2 = 1$. For $l > \sqrt{3\pi}$ a replica symmetry broken solution exists, too. Since this solution is probably the stable one, we set

$$f^{\text{RVA}}(l) := f^{\text{RSB}}(l) := -\frac{3(1 + \sqrt{2})}{(12\pi)^{1/4}} - \frac{1}{2\sqrt{l}} \left(3 + \sqrt{2} - \ln\left(8\pi^2\right)\right), \quad \text{for } l > \sqrt{3\pi}.$$

(11)

In Fig. 2 the exact and approximate averaged free energy are compared. One finds that the RVA constitutes a lower bound. This has also been observed in comparison with simulations [3, 4]. To our knowledge, this phenomenon has not yet been satisfactorily explained.

Now we turn to the calculation and discussion of the statistical properties of the Gibbs states. As can be seen from its definition, $\Omega_{\beta,L}(x)$ is invariant under a change from the $V$- to the $W$-ensemble. Therefore we may calculate all the correlation functions of the Gibbs state directly within the $W$-ensemble. The $J$-point correlation function of the scaled Gibbs state $\omega_l(s) := (8/\beta^2) \Omega_{\beta,8l/\beta^2}(8s/\beta^2)$ can be expressed due to (3) in terms of the

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Fig. 1. – Centered density of the scaled free energy $f(l)$ of the $V$-ensemble for different system sizes $l = 1/10, 1, 10, 100$. 

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Laplace transformed transition density $\tilde{p}$ as

$$\left\langle \prod_{j=1}^{J} \omega_j(s_j) \right\rangle = \frac{4^{J}}{(J-1)!} \int_{0}^{\infty} d\varrho \varrho^{J-1} \int_{-\infty}^{\infty} dw_1 \cdots dw_{J+1} \prod_{j=0}^{J} \tilde{\rho}_{s_{j+1}-s_j}(w_{j+1}, \varrho|w_j) e^{2w_j},$$

(12)

where $0 =: s_0 \leq s_1 \leq s_2 \leq \cdots s_{J+1} := l$ and $w_0 := 0$ is assumed. With the help of (6) this expression may be simplified further. Eventually we end up with a representation of the $J$-point correlation function in terms of a $(J + 1)$-fold integral of elementary transcendental functions, see [11].

Here we specialize to the most interesting situation of a large system $l \gg 1$ and large separations between the intermediate points $s_j$. As to be expected, the leading behaviour

$$\lim_{l \to \infty} l^J \left\langle \prod_{j=1}^{J} \omega_l(l\sigma_j) \right\rangle = \frac{1}{\pi \sqrt{\sigma_1(1-\sigma_1)}} \prod_{j=2}^{J} \delta(\sigma_j - \sigma_1), \quad 0 < \sigma_1, \ldots, \sigma_J < 1,$$

(13)

of the correlation function reflects the fact that the system possesses a unique ground state with probability 1. For $0 < \sigma_1 < \sigma_2 < \cdots < \sigma_J < 1$ the next-to-leading correction turns out to be

$$\lim_{l \to \infty} l^{(3J-1)/2} \left\langle \prod_{j=1}^{J} \omega_l(l\sigma_j) \right\rangle = \frac{1}{\pi \sqrt{\sigma_1(1-\sigma_1)}} \frac{(16\pi)^{(1-J)/2}}{(J-1)!} \prod_{j=2}^{J} (\sigma_j - \sigma_{j-1})^{-3/2}.$$

(14)

Fig. 2. – The main plot shows the RVA $F_\beta^{\text{RVA}}(L)$ to the averaged free energy $\langle F_\beta(L) \rangle$ for $L = 1$ as a function of temperature $1/\beta$. The vertical dashed line indicates the temperature, below which replica symmetry breaking sets in. For $1/\beta$ near 0 both curves are dominated by the logarithmic contribution in (3). Therefore the inlets show the scaled variants $f^{\text{RS}}(l)$, $f^{\text{RSB}}(l)$ and $\langle f(l) \rangle$, respectively, as a function of $1/l$. Although the leading correction of the RVA to its ground-state energy for $l \to \infty$ is of correct order $l^{-1/2}$, it is clearly seen that it has the wrong sign.
A short distance expansion given in [11] reveals that the correlation functions are analytic for small $s_j - s_{j-1}$ and finite $l$.

These results allow for a discussion of the validity of the RVA on a deeper level than does (8) because we may now check the complete structure of the probability functional of Gibbs states. Note that the average $\langle \omega(s) \rangle$ will always be a Gaussian within the replica variational ansatz used in [2] whereas it is actually $\left( \pi \sqrt{s(l-s)} \right)^{-1}$ for large systems. One might argue that this is far away from a Gaussian. However, the Gaussian form is inevitably encoded in the ansatz and thus we do not consider this a serious defect. Much more interesting is a comparison between the statistics of typical distances $\Delta = s - s'$. This has been obtained in 2 within the RVA. The result implies that the probability density $P(\Delta)$ should decrease like a Gaussian for large $\Delta$. The exact result can be obtained from $\langle \omega(s)\omega(s') \rangle$ and is given by $P(\Delta) \sim \left( 1/\sqrt{16\pi} \right) |\Delta|^{-3/2}$ for large but finite $l$ and $\Delta$. Thus the RVA severely underestimates the range of correlations. However, the most crucial feature of the RVA, which is the hierarchical structure of the ansatz, seems to be in accordance with a real property of the system, at least in a qualitative sense as we will now explain.

The geometry of typical distances may be studied by considering higher order correlations. For example, consider 3 points $0 < s_1 < s_2 < s_3 < l$ with corresponding distances $\Delta_{12}, \Delta_{13}$ and $\Delta_{23}$. If we assume $l$ and all distances to be large but finite, their joint probability density is given by $P(\Delta_{12}, \Delta_{13}, \Delta_{23}) \sim (1/32\pi)(\Delta_{12}\Delta_{23})^{-3/2}\delta(\Delta_{12} + \Delta_{23} - \Delta_{13})$. Thus for fixed $s_1$ and $s_3$ the intermediate location $s_2$ will most probably be near to one of these points. If we regard these three points as a “one-dimensional triangle” we conclude that isosceles triangles with a shorter third side are statistically preferred. In this sense, there is a weak, statistical form of ultrametricity present in the system. An ultrametric geometry also appears as a consequence of the hierarchical ansatz for the replica symmetry breaking scheme [1, 2] which thus captures an important feature of the probability functional of Gibbs states.

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