Improved perturbation theory for the Kardar-Parisi-Zhang equation

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We apply a number of schemes which variationally improve perturbation theory for the Kardar-Parisi-Zhang equation in order to extract estimates for the dynamic exponent z. The results for the various schemes show the same broad features, giving closer agreement with numerical simulations in low dimensions than self-consistent methods. They do, however, continue to predict that z=2 in some critical dimension d_c , in disagreement with the findings of simulations.

PACS number(s): 05.40.+j, 05.70.Ln, 68.35.Ja

The Kardar-Parisi-Zhang (KPZ) equation [1] is perhaps the simplest nonlinear stochastic equation of the diffusion type. Nevertheless, the large-distance scaling behavior and anomalous dimensions have not vet been understood on the basis of systematic calculational schemes, such as the renormalization group. To date, the most reliable estimates for the anomalous dimensions, obtained by direct analytic means from the KPZ equation. have come from self-consistent or pseudovariational procedures [2-4]. These approaches are, in general, rather ad hoc, and it would be useful to have a method of improving estimates and perhaps gaining some idea of their accuracy. The relative merits of procedures such as these, genuine variational procedures (by which we mean those with an associated bound) and "improvement" methods, such as "the principle of minimal sensitivity" (PMS) [5], have recently been compared for stochastic processes described by simple Langevin equations (or equivalently, Fokker-Planck equations) [6]. In this paper we extend these considerations to the KPZ equation, which can be formulated as a functional Fokker-Planck equation. It turns out that, while genuine variational techniques are not straightforward to use in this case, the application of the PMS yields improved values for the dynamic exponent z, which agree better with the results of the numerical simulation of models believed to be in the KPZ universality class.

The KPZ equation for surface growth in (d+1) dimensions with random deposition is

$$\dot{h}(\mathbf{x},t) = \nu_0 \nabla^2 h + g(\nabla h)^2 + \eta(\mathbf{x},t), \tag{1}$$

where the single-valued function $h(\mathbf{x},t)$ represents the interface and \mathbf{x} is a d-dimensional vector. The subscript 0 on surface tension ν_0 and noise strength D_0 (below) is used to distinguish these bare parameters from the effective (renormalized) ones to be introduced later. The noise $\eta(\mathbf{x},t)$ is Gaussian distributed with zero mean $\langle \eta(\mathbf{x},t) \rangle = 0$ and δ -function correlations

$$\langle \eta(\mathbf{x},t)\eta(\mathbf{x}',t')\rangle = 2D_0\delta(\mathbf{x}-\mathbf{x}')\delta(t-t').$$
 (2)

Equivalently the noise may be specified in terms of the probability density functional

$$\mathcal{P}[\eta] \sim \exp\left\{-(4D_0)^{-1}\int dt\int d^dx \left[\eta(\mathbf{x},t)\right]^2\right\}.$$
 (3)

The KPZ equation (1) can then be taken as a transformation of variables $\{\eta(\mathbf{x},t) \to h(\mathbf{x},t)\}$ [7], which leads to the following probability distribution of the h field:

$$\mathcal{P}[h] \sim \left| \operatorname{Det} \frac{\partial h(\mathbf{x}, t)}{\partial \eta(\mathbf{x}', t')} \right| \exp \left\{ -\frac{1}{4D_0} \int dt \int d^d x [\dot{h} - \nu_0 \nabla^2 h - g(\nabla h)^2]^2 \right\}. \tag{4}$$

The Jacobian above can be shown to be h independent; it plays no role in what follows and will be dropped. Introducing the response field $\tilde{h}(\mathbf{x},t)$ [8] yields the distribution of the h and \tilde{h} fields as $\mathcal{P}[h,\tilde{h}] \sim \exp\{\mathcal{S}_0[\tilde{h},h]\}$, where

$$S_0[\tilde{h}, h] = \int dt \int d^dx \Big\{ D_0 \tilde{h}^2(\mathbf{x}, t) - \left[\dot{h} - \nu_0 \nabla^2 h - g(\nabla h)^2 \right] \tilde{h}(\mathbf{x}, t) \Big\}.$$
 (5)

Note that the \tilde{h} 's are actually imaginary. Fourier transforming the fields gives

$$S_{0}[\tilde{h}, h] = \int \frac{d\omega}{2\pi} \int \frac{d^{d}k}{(2\pi)^{d}} \left[D_{0}\tilde{h}(\mathbf{k}, \omega)\tilde{h}(-\mathbf{k}, -\omega) - \left(\nu_{0}\mathbf{k}^{2} - i\omega\right)h(\mathbf{k}, \omega)\tilde{h}(-\mathbf{k}, -\omega) \right]$$

$$-g \int \frac{d\omega}{2\pi} \int \frac{d^{d}k}{(2\pi)^{d}} \int \frac{d\omega'}{2\pi} \int \frac{d^{d}k'}{(2\pi)^{d}} [\mathbf{k} \cdot \mathbf{k}']h(\mathbf{k}, \omega)h(\mathbf{k}', \omega')\tilde{h}(-\mathbf{k} - \mathbf{k}', -\omega - \omega').$$

$$(6)$$

The problem is completely solvable in the absence of the nonlinear term (g=0) [9], but one cannot access the strong-coupling fixed point through perturbation and the renormalization group. With these approaches ruled out, we turn to approximation techniques such as variational methods and related procedures. But just what kind of schemes are available?

Before answering this question, let us make the first step toward a variational scheme by adding and subtracting an effective action functional $S_{\text{eff}}[\tilde{h}, h]$,

$$\mathcal{P}[h, \tilde{h}] \sim \exp \left\{ \mathcal{S}_{\text{eff}} + \lambda \left(\mathcal{S}_0 - \mathcal{S}_{\text{eff}} \right) \right\},$$
 (7)

where λ serves as a counting device and will eventually be set to 1. The most satisfactory approach would be a genuine variational scheme. Many of these are based on some version of the inequality $e^x \geq 1+x$, which can be extended to

$$e^x \ge \sum_{n=0}^{2N-1} \frac{x^n}{n!}.$$
 (8)

It is tempting to expand $\exp{\{\lambda(S_0 - S_{\text{eff}})\}}$ and invoke this inequality; however, it does not hold, as the \tilde{h} 's are imaginary and the above inequality applies to real x only.

Since the existence of an imaginary part to $S_0[\tilde{h},h]$ appears to be the stumbling block, perhaps it would be better to tackle the problem prior to introducing the response field. The inequality would hold, but a new problem arises. While one can proceed with a perturbation expansion around the bare quadratic terms in (4), introducing variational quadratic terms to serve as a basis for perturbation rearranges the series, and one loses the property that divergences associated with the disconnected diagrams cancel order by order. These divergences render the inequality useless.

There are other genuine variational schemes based on the differential form of the Fokker-Planck equation [6] and applicable to problems with a finite number of degrees of freedom. But they too are plagued with divergence problems when applied to a field theory. On the other hand, techniques are available that involve similar computational steps to the variational one, although the philosophy is rather different. In particular, they do not involve bounds such as those given by (8). These techniques can be formulated by choosing a form for the effective action \mathcal{S}_{eff} , which (i) is quadratic (for calculational

convenience) and (ii) has the same structure as quadratic terms in the bare action S_0 , but with $\nu_0 q^2 \to \nu_{\mathbf{q}}$ and $D_0 \to D_{\mathbf{q}}$; that is, with the bare surface tension and bare noise strength replaced by their effective, or renormalized, counterparts:

$$S_{\text{eff}}[\tilde{h}, h] = \int \frac{d\omega}{2\pi} \int \frac{d^{d}k}{(2\pi)^{d}} \Big[D_{\mathbf{k}} \tilde{h}(\mathbf{k}, \omega) \tilde{h}(-\mathbf{k}, -\omega) - (\nu_{\mathbf{k}} - i\omega) h(\mathbf{k}, \omega) \tilde{h}(-\mathbf{k}, -\omega) \Big]. \tag{9}$$

The simplest scheme is probably the one pioneered by Edwards [10,2], where one chooses the functions $\nu_{\mathbf{k}}$ and $D_{\mathbf{k}}$ to be the "exact" (but as yet unknown) surface tension and noise strength, respectively. When $\mathcal{P}[h, \tilde{h}]$ is expanded in λ , the zeroth-order term will give the correct result (by construction) and hence the rest of the perturbation expansion (terms in $\lambda, \lambda^2, \ldots$) will have to be identically zero. This, together with a scaling ansatz for the response and correlation functions, gives values for the exponent z [2], which we will later compare to our findings. This scheme has been called "fastest apparent convergence" or FAC.

The approach based on the PMS is calculationally similar to those already described — it involves the same diagrams, since one is expanding the same quantity about the same zeroth-order form (9), but now the rationale is different. The response or correlation function being calculated should not depend on $\nu_{\bf q}$ or $D_{\bf q}$, since these were introduced artificially and are not part of the "real" problem; however, any truncated expansion does depend on them. One then imposes a stationarity condition on the expansion to determine the result that displays the least dependence on them. Thus one asks that the expansion mimic as best as possible one feature of the true solution, its insensitivity to these variational terms, with the hope that other features will be mimicked as well.

As we have stressed, all the schemes discussed so far are based on a perturbative calculation in the parameter λ . The structure of the perturbation expansion and the diagrams is essentially that given by Forster, Nelson, and Stephen [11], except that these authors were expanding in g and we are expanding in λ . Thus we have quadratic, as well as cubic, terms in our "interaction" term and hence have terms odd in λ in addition to the more familiar $O(\lambda^2)$ terms of Ref. [11].

A perturbative calculation of $\langle |h(\mathbf{q},\omega)|^2 \rangle$ to $O(\lambda^2)$ yields

$$\langle |h(\mathbf{q},\omega)|^{2} \rangle = \frac{2D_{\mathbf{q}}}{(\nu_{\mathbf{q}}^{2} + \omega^{2})} + \lambda \left[\frac{2(D_{0} - D_{\mathbf{q}})}{(\nu_{\mathbf{q}}^{2} + \omega^{2})} - \frac{4D_{\mathbf{q}}\nu_{\mathbf{q}} (\nu_{0}q^{2} - \nu_{\mathbf{q}})}{(\nu_{\mathbf{q}}^{2} + \omega^{2})^{2}} \right]$$

$$+ \lambda^{2} \left[\frac{2D_{\mathbf{q}} (\nu_{0}q^{2} - \nu_{\mathbf{q}})^{2} (3\nu_{\mathbf{q}}^{2} - \omega^{2})}{(\nu_{\mathbf{q}}^{2} + \omega^{2})^{3}} - \frac{4(D_{0} - D_{\mathbf{q}})\nu_{\mathbf{q}} (\nu_{0}q^{2} - \nu_{\mathbf{q}})}{(\nu_{\mathbf{q}}^{2} + \omega^{2})^{2}} \right]$$

$$+ \frac{4g^{2}}{(\nu_{\mathbf{q}}^{2} + \omega^{2})} \int \frac{d^{d}k}{(2\pi)^{d}} \frac{\left[\mathbf{k} \cdot (\mathbf{k} + \mathbf{q}) \right]^{2} D_{\mathbf{k}} D_{\mathbf{k} + \mathbf{q}} (\nu_{\mathbf{k}} + \nu_{\mathbf{k} + \mathbf{q}})}{(\nu_{\mathbf{k}} + \nu_{\mathbf{k} + \mathbf{q}})^{2} + \omega^{2}}$$

$$- \left\{ \frac{8g^{2} D_{\mathbf{q}}}{(\nu_{\mathbf{q}} - i\omega) (\nu_{\mathbf{q}} + i\omega)^{2}} \int \frac{d^{d}k}{(2\pi)^{d}} \frac{\left[\mathbf{k} \cdot \mathbf{q} \right] \left[\mathbf{k} \cdot (\mathbf{k} + \mathbf{q}) \right] D_{\mathbf{k}}}{\nu_{\mathbf{k}} (\nu_{\mathbf{k}} + \nu_{\mathbf{k} + \mathbf{q}} + i\omega)} + \text{c.c.} \right\} \right],$$

$$(10)$$

where the internal frequency integral has been carried out.

There are various ways to proceed at this stage. We want the calculation to be simple without sacrificing any physics, so let us focus on the large-distance scaling behavior. Response and correlation functions calculated from (4) would be invariant under the scale transformation $\{\mathbf{x} \to b\mathbf{x}, \ t \to b^zt, \ h \to b^xh\}$ if the parameters scaled like $\{\nu \to b^{z-2}\nu, D \to b^{-d-2}\chi + zD, g \to b^{z+\chi-2}g\}$. We build these scalings into our effective surface tension and noise strength by choosing

$$\nu_{\bf q} = Aq^z \text{ and } D_{\bf q} = Bq^{-d-2\chi+z}.$$
(11)

We also impose the exponent relation $z + \chi = 2$ due to the Galilean invariance [11,12]. In what follows we will retain only the leading scaling behavior; thus the bare terms ν_0 and D_0 will no longer appear.

Two natural ways of simplifying Eq. (10) are first integrating over ω and second setting $\omega = 0$. These yield

$$\int \frac{d\omega}{2\pi} \langle |h(\mathbf{q},\omega)|^2 \rangle = \frac{B}{A} \{ 1 + \lambda^2 u I_1(d,z) -2u I_2(d,z) \} |\mathbf{q}|^{-\Gamma},$$
(12)

$$\langle |h(\mathbf{q},0)|^2 \rangle = \frac{2B}{A^2} \{ 1 + \lambda + \lambda^2 [1 + uJ_1(d,z) - 4uJ_2(d,z)] \} |\mathbf{q}|^{-z-\Gamma},$$
(13)

respectively, where $\Gamma = d + 4 - 2z$, $u = 2g^2B/A^3$,

$$I_{1}(d,z) = \int \frac{d^{d}p}{(2\pi)^{d}} \frac{\left[\mathbf{p} \cdot (\mathbf{p} + \mathbf{1})\right]^{2} |\mathbf{p}|^{-\Gamma} |\mathbf{p} + \mathbf{1}|^{-\Gamma}}{(1 + |\mathbf{p}|^{z} + |\mathbf{p} + \mathbf{1}|^{z})}, \quad (14)$$

$$I_2(d,z) = \int \frac{d^d p}{(2\pi)^d} \frac{\left[\mathbf{p} \cdot \mathbf{1}\right] \left[\mathbf{p} \cdot (\mathbf{p} + \mathbf{1})\right] |\mathbf{p}|^{-\Gamma}}{(1 + |\mathbf{p}|^z + |\mathbf{p} + \mathbf{1}|^z)}, \tag{15}$$

and $J_i(d, z)$ is the same as $I_i(d, z)$ (i=1,2), except that the term in the denominator $(1 + |\mathbf{p}|^z + |\mathbf{p} + \mathbf{1}|^z)$ is replaced by $(|\mathbf{p}|^z + |\mathbf{p} + \mathbf{1}|^z)$.

When carrying out the PMS scheme we ask that the correlation functions (12) and (13) be insensitive to the artificially introduced quantities (11). Since $\nu_{\mathbf{q}}$ and $D_{\mathbf{q}}$ were assumed to have power-law forms, they are, apart from the amplitudes A and B, completely characterized by the exponent z. Thus, implementing the PMS in this case entails requiring that the expressions (12) and (13) be independent of z. There is, however, a subtlety here. One cannot apply the PMS to a function and vary with respect to a single parameter, as that results in an overdetermination. Either we perform a functional variation, or we apply the method to a q-independent quantity. Here we choose to vary with respect to z alone, so we should be analyzing a correlation function that has a qindependent scaling form. One possibility is to treat correlation functions of the type $\langle (\nabla^{\alpha} h)^2 \rangle$, which in **q** space reads $|\mathbf{q}|^{2\alpha} \langle |h(\mathbf{q},\omega)|^2 \rangle$, rather than $\langle |h(\mathbf{q},\omega)|^2 \rangle$. Here we choose α so that the analogs of (12) and (13) are **q** independent. Differentiating these expressions with respect to z gives

scheme 1
$$\partial_z [I_1(d,z) - 2I_2(d,z)] = 0,$$
 (16)

scheme 2
$$\partial_z [J_1(d,z) - 4J_2(d,z)] = 0,$$
 (17)

respectively.

An alternative to starting from the full correlation function $\langle |h(\mathbf{q},\omega)|^2 \rangle$ is to extract the parts of this function that contribute to the renormalization of the noise strength. This is achieved by amputating the two external legs on the graphs for the correlation function; that is, removing two factors of $G(\mathbf{q},\omega)$ from (10). The resulting forms for the leading scaling behavior resemble (12) and (13), but without the terms involving the integrals I_2 and J_2 . Applying the PMS to the noise strength gives equations analogous to (16) and (17):

scheme 3
$$\partial_z [I_1(d,z)] = 0,$$
 (18)

scheme 4
$$\partial_z [J_1(d,z)] = 0.$$
 (19)

To find z from (16)–(19) we have to evaluate integrals such as (14) and (15) for a range of values of z. Going over to d-dimensional spherical polar coordinates, the integrals may be reduced to double integrals, depending on the parameters d and z. We have taken great care in numerically integrating the double integrals that give $\partial I_i/\partial z$ and $\partial J_i/\partial z$, (i=1,2), since there are potential singularities at $\mathbf{p}=\mathbf{0},-\mathbf{1}$ and as $|\mathbf{p}|\to\infty$. In the first two cases the integrals converge if z>1, which is always true. The singularities at large $|\mathbf{p}|$ are more severe: integrals of the type (14) only exist if z<(d+4)/3 and those of the type (15) if $z\leq 2$. In the latter case a naive analysis might suggest that the integral only exists when z<1, but the leading large $|\mathbf{p}|$ term vanishes by $\mathbf{p}\to -\mathbf{p}$ symmetry.

Based on these considerations, we have searched for solutions of (16)–(19) for parameter values 1 < z < (d+4)/3 for $1 \le d \le 2$ and $1 < z \le 2$ for $d \ge 2$. Within this parameter range there are integrable singularities that numerical integration routines find difficult to cope with. For this reason, we have used various transformations that remove these integrable singularities, as well as different routines, in order to check our computations. Note that while schemes 3 and 4 seem to admit solutions with z > 2, it is easy to check that the subleading nonscaling terms that were discarded to obtain (12) and (13) are only subdominant if z < 2. Thus the entire method is dependent on this bound being respected.

For schemes 3 and 4, we readily find solutions, and the resulting values of z are reported in Table I below. We find no solutions to schemes 1 and 2 as presented above. However, the PMS methodology asserts that if the point of minimal sensitivity is not found by setting the derivative equal to zero, one should next seek to minimize the derivative, and so on [5]. In this light we revise these schemes and look at higher derivatives. Scheme 2 has a solution when the second derivative is set to zero and the corresponding values of z are reported in the table. On the other hand, we have seen no evidence for a solution to scheme 1 (in d=2) upon examining the second and third derivatives.

The simulation results included in the table are from the hypercube-stacking model simulated in dimensions

$d \mid$	Simulation	SE	BC	Scheme 2	Scheme 3	Scheme 4
1	$1.500{\pm}0.001$	1.500	1.500	1.424	1.420	1.465
2	$1.613{\pm}0.003$	1.705	1.667	1.582	1.553	1.621
3	$1.695{\pm}0.007$	1.920	1.862	1.740	1.682	1.769
4	$1.77{\pm}0.02$			1.909	1.810	1.914
d_c		3.2	3.6	4.4	5.4	4.6

TABLE I. Values of the dynamic exponent z.

d=1,2,3 [13] and the restricted solid-on-solid model, simulated up to dimension d=7 [14], both believed to belong to the KPZ universality class. The measurements of the exponent β , which governs the early growth, agree between the models for d=1,2,3. In the table we list the corresponding value for the dynamic exponent $z=2/(\beta+1)$ and include the larger reported error bar. The data for d=4 showed large fluctuations and finite-size dependence, making it more difficult to establish accurate estimates of the exponents [14].

Schwartz and Edwards (SE) [2] adopted the FAC approach, determining z by setting the terms of $O(\lambda)$ and higher in (12) to zero; the outcome of this procedure is included in the column labeled SE. The column labeled BC contains the findings of Bouchaud and Cates [3], who pursued a self-consistent approach. Actually the latter can also be formulated using the FAC criterion; the only difference being that SE integrates over ω while BC sets $\omega = 0$. Incidentally, the equations obtained by BC [3] can also be derived as part of a functional PMS variation; but one in which scaling is still ultimately put in by hand, and not deduced.

The values for z furnished by the PMS schemes (2–4) follow the same general pattern: they fall below the exact value of z=3/2 in d=1 by a few percent; they then increase as d increases and eventually reach z=2 in some critical dimension d_c (listed in the table) in disagreement with the simulation results. Note that the self-consistent methods contain enough of the correct structure to yield the exact value of z=3/2 in d=1. The PMS approach uses this same structure and information but in a very

different way, and the exact result in d=1 is no longer guaranteed. However, for $d \geq 2$, the PMS schemes are more in line with the simulation results.

In this paper we have applied the PMS to obtain improved estimates for the exponent z in the KPZ equation. The ideas discussed here could be extended in a number of ways. Besides the obvious, but tedious, course of going to higher order in the perturbation, one could adopt a more general (though still Gaussian) form for (9), allowing for a frequency-dependent noise strength $D_{\mathbf{k},\omega}$ or for a more general functional form $G^{-1}(\mathbf{k},\omega)$ in place of the response $\nu_{\mathbf{k}} - i\omega$. This has proved successful within the self-consistent approach, where a more sophisticated Ansatz for the response function in Ref. [4] led to improved results for z. It would be interesting to see if more general Ansätze such as these would similarly improve on the estimates presented here. A more ambitious calculation would be to apply the PMS to the function (10) without assuming scaling. In the absence of a renormalization group treatment of this problem, approaches such as these may be the most promising ways toward an understanding of the anomalous large-distance behavior of the KPZ equation.

We wish to thank J. P. Doherty for useful discussions and the Isaac Newton Institute for Mathematical Sciences, where this work was begun, for its hospitality. T.B. acknowledges the support of the Engineering and Physical Sciences Research Council under Grant No. GR/H40150.

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