Reply to "Comment on 'Renormalization-group theory for the phase-field crystal equation' "

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In a recent Comment [Y. Shiwa, Phys. Rev. E **79**, 013601 (2009)], Shiwa points out that our multiple-scales analysis of the Van der Pol equation [Appendix of Phys. Rev. E **74**, 011601 (2006)] contained an error, and thus there may be no ordering ambiguity for renormalization and differentiation operations, as we had proposed for the phase-field crystal equation and other conservation laws. The Van der Pol analysis was indeed incorrect, and while his Comment casts doubt over our treatment of the multiple-scales analysis of the phase-field crystal (PFC) equation, there is no substantial change to our renormalization (RG) group results or simulations of the PFC model. This example highlights the merits of the RG approach to singular perturbation problems: the RG method is more mechanical and requires less user-insight than traditional methods.

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In an earlier paper [1], we attempted to derive the amplitude equation to the phase-field crystal (PFC) model—a conservation law [2]—using several variants of the renormalization group (RG) method and compared the results obtained thereby with the result derived from a benchmark multiple-scales (MSs) analysis of the same model. We noted a discrepancy between the RG results and the MSs results, viz. the MSs analysis yielded certain extra higher-order terms in the amplitude equation which were not captured by either of the RG methods. We have since verified that these terms have virtually no bearing over our simulations of the PFC equation. In our paper, we attempted to resolve this apparent mismatch by proposing a different ordering of the renormalization and differentiation operations (see [1] for details) in the RG method that led to agreement with the MSs results. We attributed this ordering ambiguity to the presence of the conservation law.

In his Comment Shiwa has, however, argued that there is no need for this reordering, claiming an error in our MSs analysis. The Comment has two parts, and these need to be considered separately.

(1) The Comment points out an error in the Appendix of our original paper in the derivation of the amplitude equation for the Van der Pol oscillator using MSs. The author states that we ignored an extra time scale inherent to this problem, as a result of which our derivation using MSs did not match the derivation using the proto-RG method. Based on this he concludes that there is no need for the modification we suggested for the RG method (renormalization before differentiation) as applied to the Van der Pol oscillator in the Appendix of our paper. We agree completely with this point. We made an error in the MSs calculation, and if we had not done so, the original RG calculation would have easily given the correct result.

(2) The Comment goes on to argue that the MSs scale result for the (one-dimensional) PFC equation that we derived in our paper must also be incorrect—and that had the MSs analysis been correctly done, our result would have agreed with the standard RG calculation derived in the paper. Thus there would not be a need to make any modification of the standard RG calculation. Actually, as much as we would like this to be the case (the senior author on our paper was one of the original developers of the RG method), the Comment does nothing to prove this, although it does point out one area of doubt in our MSs calculation: the neglect of a zero mode, arising from the conservation law to which we had already drawn attention. We agree that this neglect casts doubt on the MSs calculation that we used as a standard of comparison for our RG calculations, and presume that if the RG calculation were compared with the correct MSs calculation, there would be agreement without any need for modifying the order of renormalization and differentiation. However, Shiwa does not show this in his Comment.

While we welcome Shiwa's identification of our error in the multiple-scales analysis, we would like to clarify a couple of points.

(I) We point out that there is a disconnect between the calculation done in the Appendix (the Van der Pol oscillator) and the calculation on the PFC equation: the Van der Pol oscillator does not exhibit the conservation law which we already recognized in our paper was causing a problem in the derivation of amplitude or RG equations. The calculation error made in the Appendix using the MSs method had nothing to do with the main issue addressed in our paper, namely, the coarse graining of the PFC equation. In other words, we made two separate errors in using the MSs method.

(II) More importantly, the Comment does not report a full RG calculation and comparison with the correct MSs calculation on the PFC equation; i.e., this is still an open question requiring a more complete treatment. The author himself says as much, in the closing of his Comment. We look forward to a complete resolution of this question.

We conclude by noting that this episode highlights the superiority of RG methods over existing singular perturbation theory techniques, such as the MSs method, which require delicacy in order to be correctly operated.

[1] B. P. Athreya, N. Goldenfeld, and J. A. Dantzig, Phys. Rev. E **74**, 011601 (2006).

[2] The PFC equation describes the evolution of the time-averaged local atomic density field in the material. An interesting property of the PFC equation is that under appropriate boundary conditions, e.g., periodic boundaries, the density field when spatially averaged over the physical domain remains constant in time, since for equal influx and outflow of atoms, the mass of the system must be conserved.

Comment on "Renormalization-group theory for the phase-field crystal equation"

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Athreya, Goldenfeld, and Dantzig [Phys. Rev. E **74**, 011601 (2006)] claim that the current implementation of the renormalization-group method neglects the proper ordering of renormalization and differentiation. Their analysis is, however, based on the wrong multiple-scales method results.

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The phase-field crystal (PFC) model [1] is the continuum approach that is promising in successfully treating many nonequilibrium dynamics arising during materials processing. On the other hand, the amplitude equation approach that describes the slowly varying amplitudes of the order parameter field always plays an important role in theories of pattern formation in general outside of equilibrium. Therefore it is quite natural that the amplitude equation (AEq) has been proposed [2] as a coarse-grained version of the PFC model. We shall call the proposed equation the heuristic AEq since the method to derive it is phenomenological and rather heuristic.

In a recent paper [3], Athreya, Goldenfeld, and Dantzig (AGD) employed various singular perturbation methods to see if the heuristic AEq could be derived from systematically coarse graining the PFC equation. More specifically they used the multiple-scales (MSs) method and variants of the renormalization group (RG). They assume that the criterion upon which to test the accuracy of a theory is the method of MSs. Thus if one method yields the result which is closer to the MSs result than the other, then that method is deemed more correct. The net outcome of their calculations is that none of the current RG methods agrees with the MSs solution.

Confronted with this difficulty and in order to get the RG calculation to agree with the MSs calculation, AGD claimed that one has to depart from the conventional RG procedure originally developed by Chen *et al.* in [4]. Namely, operator ordering in the RG procedure is to be treated properly, and that the amplitude must be renormalized before the differential operation is performed upon the amplitude in exactly the opposite order of operations which is employed in the current RG methods [4–6]. They then showed that, with this remedy implemented, the (proto-)RG method produces the same answer as the method of MSs; to this finding we will return below. To justify the generality of the proposed RG prescription, they then used the Van der Pol oscillator as an example. The explicit results of the proto-RG which is modified as prescribed as above and the MSs calculations were given, and showed that they agreed with each other.

However, the MSs solution given by AGD for the Van der Pol problem omitted a needed extra time scale. In fact, the three-time expansion is necessary to kill the secular terms that appear in their calculations [7], while they erroneously used the two-timing MSs expansion by starting their calculations with the statement: "It is known that the scaling $\tau = \epsilon t$ works for this problem [30]" ([30] being the reference cited in [3]). Redone with the correct number of time scales, the amplitude equation obtained from the MSs method becomes

$$\frac{dA}{dt} = \epsilon\frac{A}{2}(1-|A|^2) - \epsilon^2\frac{i}{8}A\left(1-4|A|^2+\frac{7}{2}|A|^4\right) + O(\epsilon^3), \tag{1}$$

which agrees with the unmodified proto-RG result [5]. Thus the very example that AGD have chosen for their calculations shows that the conventional RG methods should not be modified as advocated by them, for ordinary differential equations, to say the least. Moreover, it is rather an easy exercise to prove that all the conventional RG methods give the identical result, which agrees exactly with the MSs solution (1).

The MSs result for the PFC equation due to AGD has overlooked an important physics. We wish to point out here that the conservation law inherent in the PFC equation implies the existence of neutral modes at zero wave number. The important point to remember is that in the vicinity of the instability to a cellular structure of finite wave number (k_c), the amplitude of slow neutral modes couples to that of the critical modes at k_c and modifies the dynamics significantly. The well-known example is the case of vertical vorticity modes in Rayleigh-Bénard convection with stress-free boundary conditions [8]. Unfortunately, the MSs solution by AGD fails to take these slow modes into account and hence cannot be right. Indeed, the standard MSs analysis shows that the neutral mode generates, e.g., an additional term proportional to

$$(1-\mathcal{L}_{1D})AB \tag{2}$$

to the MSs solution of AGD [i.e., Eq. (46) in [3]; we have used the same notations as therein], where B is the amplitude of the neutral mode. See also Ref. [23] cited by AGD [3]. As already described above, AGD employed the method of MSs as a benchmark for accuracy of theory. Since the MSs solution that AGD employed is thus incorrect, we are inevitably led to the conclusion that the proposed amendment to the current RG methods is unfounded. We remark in closing that although the method of MSs thus could not justify the heuristic AEq, to reproduce the correct MSs solution alluded to above by the now standard (or revised) RG method is another story from the context of the present discussion. Certainly, the RG calculation of AGD itself needs to be improved to take the zero mode into account before any conclusion can be reached.

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