Feedback for Written Portion of PhD Prelim Exam for Sam Nittala

1   Overall Assessment

The committee feels that the written document should be considered a **pass** and that the candidate should proceed to the oral portion of the preliminary exam.

2   Expectations and Suggested Study Materials

- "Statistical Physics" by Landau and Lifshitz (thermodynamics of phase coexistence)

- "Principles of Condensed Matter Physics" By P.M Chaikin and T.C Lubensky, Cambridge University Press (elasticity and hydrodynamics of solids)

- "Phase Equilibria, Phase Diagrams and Phase Transformations: Their Thermodynamic Basis", by Matts Hillert, Cambridge University Press (phase coexistence and vacancies)

- "Phase Field Modelling in Materials Science and Engineering", by N. Provatas and K. Elder, Springer Verlag (interface properties and phase field theories)

- Of course, the committee will be asking around your research in general, so please be sure to brush up on relevant references (e.g., some of the more important ones that you cite in the document!)

3   Detailed Comments and Questions

3.1   Adrian

The write-up is well-organized and seems to cover the basic ideas that will be pursued. There is a clear structure regarding the candidate's PhD projects and a clear timeline with a path towards a degree. My only slight complaint is that the document moved into information for specialists *very* quickly. I encourage the candidate to include a little more introductory material during the presentation.

A few items for the candidate to address during the presentation (or perhaps in the first few questions if the presentation doesn't adequately cover these points):

- It was fun to see a lot of the same math that one sees in cosmology! For instance, we also express our field in terms of the dimensionless fluctuation (except we call it δ rather than n). Similarly, we also consider the regime of small fluctuations like some of the expansions done on page 3. But my understanding is that during a phase transition, it's not necessarily appropriate to approximate the fluctuations as being small. Can you help me understand why this is ok?

- Another bit of common terminology with cosmology is the notion of a topological defect. Can you define a topological defect?

- You say before Equation 5 that "for my purposes, it will be given by an envelope of Gaussian peaks". Can you justify this?

Below are some sample questions that I *may* ask during the exam (note that committee members also reserve the right to ask similarly scoped questions). Being a non-specialist on the committee, I will focus on basic thermodynamics and statistical mechanics at the undergraduate level:

- In Section 2.1, you talk about "the" free energy. Can you talk generally about the concept of free energy, discussing how it is useful and how it differs from the internal energy? Also discuss different types of free energy (e.g., Helmholtz free energy, Gibbs free energy, etc.), how they're defined, and how they're useful.

- What's the difference between a first-order phase transition and a second-order phase transition?

- Define what one means by "correlation function". Discuss some of the intuition behind correlation functions and how they're used (more generally than just the calculations in the prelim document).

- What is Maxwell's construction and how is relevant to phase transitions?

3.2 Hong

This is a well-written document by the author, the research problems are interesting, and the prelim exam can move forward. The following are questions which may be asked during the exam.

- Why Stefan problem (moving boundary problem) is hard to solve numerically?

- In the SI models, thermodynamic boundary conditions (like Gibbs-Thompson relation) are explicitly applied. In PF models and going to the sharp interface limit, can you derive such thermodynamic boundary conditions? Which is more "fundamental", SI or PF ?

- At large solidification speed, "Stefan problem breaks down, in the sense that local equilibrium at the solid-liquid interface no longer holds...". This is generally true since at far from equilibrium, things like free energies may not apply. Please explain why PF models continue to work. In Eq.(1) or (4), there is still a free energy functional F. At far from equilibrium, shouldn't we solve a nonequilibrium distribution function satisfying some master equations?

- It seems Eq.(5) is important for obtaining a solid structure. For a co-valent crystal structure (like a semiconductor), is the two-point structure factor enough or one needs some higher-point correlations?

- Following above, can you please remind us why the structural factor in the liquid side can determine the structure across the phase boundary at the solid side?

- Eq.(9) is interesting but I didn't have time to read Ref.[36] for its derivation. Please explain why the quantity N_b depends on the curl of the stress tensor? It is vaguely reasonable, is it obvious?

- Intuitively, after the flat solid/liquid interface becomes unstable, undulations appear (cusps?) which are eventually driven to structures like dendrites. At large interface speed, such undulations do not have time to relax – they get trapped, leading to dislocation. Is this picture correct?

- What determines the banding periodicity in Fig.5b?

3.3 Dave

The proposal is good enough to proceed to the oral exam. It is well written and I have no comments on the text. A few sample questions:

- Is there a Reynold's number-type figure that dictates whether a liquid/solid interface becomes likely to exhibit cusps evolving from a planar interface, at a given speed?

- What are the experimental techniques by which such dislocations can be identified in metals?

- What are the experimental techniques that can observe the dynamic formation of a defect? Are there any?

- When is a two dimensional simulation representative of a 3D material? What are the limitations of that?

3.4 Nik

Excellently organized and written with a sold plan to complete papers and thesis. The written document is good to proceed to the prelim.

Specific feedback on the prelim document to address during the presentation:

- State how different modes in Eq. 8 may also be used to model more complex crystallography.

- Indicate, briefly, how Eq. 4 changes if the scaling of F is done by $k_B * T_0 * \rho_0$ (T_0 = reference temperature)

- Perhaps call the common tangent as the "Maxwell equal area construction", more familiar to physicists

- Have the formula in footnote 8 ready for the prelim.

Four questions closely related to those I may ask in the Q/A portion of the prelim:

- Derive the Gibbs-Duhem relationship for a multi-component system and use it to explain the Gibbs phase rule.

- Derive the thermodynamic relations for determining the two-phase coexistence region of the phase diagram of a pure material in (ρ-T) space (ρ is density, T is temperature). Assume the system has a constant volume (V) and contains a constant number of particles (N).

- Derive an expression for the equilibrium fraction of vacancies in a crystalline solid of pure material containing N atoms at temperature T and fixed pressure p.

- Derive the connection between the interface temperature and its local velocity in the regime of high vacancy trapping using Model A as a model to describe the kinetics for the phase transformation