Energy Driven Pattern Formation in Planar Dipole–Dipole Systems

Andrew J. Bernoff & Jaron P. Kent-Dobias

Harvey Mudd College, Claremont, CA

Introduction

Many two-dimensional fluid systems exhibit a dipole–dipole interaction between fluid particles. The competition between short-range cohesive fluid forces and the long-range repulsive dipole–dipole force creates intricate structures. These systems include ferrofluid confined to a Hele-Shaw cell and Langmuir films, images of which are shown in Fig. 1(a–b) and Fig. 1(c–d), respectively.

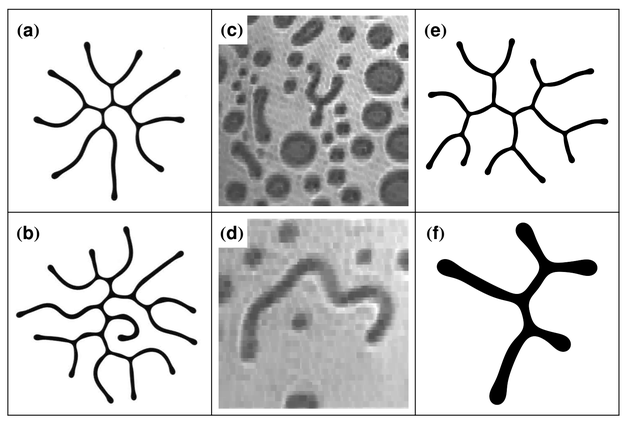

Figure 1: Examples of planar dipole–dipole systems. (a–b) Ferrofluid confined to a Hele-Shaw cell. From D. P. Jackson. (c–d) Langmuir films. From E. K. Mann. (e–f) Results of our numeric model.

Our work models these dipole-mediated systems using energy minimization. First, we build a description for the energy of any dipole-mediated system which depends on only one parameter, called Λ, independent of the microscopic details of the particular system under consideration. We numerically model pattern formation in these systems via energy minimization. We find very few energy-minimizing domain morphologies, but adding a small random energy background recovers the rich diversity of shapes seen in experiment. Examples of these results can be seen in Fig. 1(e–f). Finally, we use domain data generated by our numerics to form and test a simple model for determining Λ in terms of the domain's perimeter and morphology.

Energy Formalism

In general, the energy of a dipole-mediated domain can be written as

$$E = \lambda\ell + \frac{\mu^2}{2}\iint_\Omega\iint_\Omega \frac{g(\|\mathbf{r}-\mathbf{r}'\|)}{\|\mathbf{r}-\mathbf{r}'\|^3}\,\mathrm{d}A'\,\mathrm{d}A$$

The first term is the interfacial energy, characterized by the *line tension* λ and proportional to the *perimeter* ℓ. The second term is the dipole–dipole term, characterized by the *density of dipoles* μ and the *radial distribution function* $g(r)$, which gives the distribution of particle centers about a given fluid particle. The radial distribution function normally depends in a complex way on the geometry and packing of the fluid particles and can vary wildly from system to system. However, it has properties which are identical for any fluid: it must vanish at the origin, and must approach one within some small, particle-scale distance Δ. In most systems, Δ is much smaller than the characteristic domain size, which for a domain of area A is $R = \sqrt{A/\pi}$. Asymptotic analysis yields an approximate energy which, in a dimensionless form, is

$$F = \Lambda L - \frac{1}{2}\oint_{\partial\Omega}\int_{-\frac{L}{2}}^{\frac{L}{2}}\left[\frac{\hat{\mathbf{n}}(s)\cdot\hat{\mathbf{n}}(s+\sigma)}{\|\boldsymbol{\rho}(s)-\boldsymbol{\rho}(s+\sigma)\|}-\frac{1}{|\sigma|}\right]\mathrm{d}\sigma\,\mathrm{d}s - L\log L$$

Here, $F \equiv E/\mu^2 R$, $\Lambda \equiv \frac{\lambda}{\mu^2} - \log\frac{l}{\Delta}$, $L \equiv \ell/R$, $\boldsymbol{\rho} \equiv \mathbf{r}/R$, and $\hat{\mathbf{n}}$ is the unit normal vector to the parameterization $\mathbf{r}(s)$. This expression for the energy of a dipole-mediated system depends only on one parameter, Λ, and the shape of the system's boundary.

One can minimize the energy exactly for few problems using this formula. One such problem is the energy of a rectangle. We find that, in the limit of large negative Λ, the perimeter of an energy-minimizing rectangle goes as $L_{\text{rec}} = 2\pi e^{-(\Lambda+1)}$, and its width goes as $w_{\text{rec}} = e^{\Lambda+1}$. These formulae will later be important in the formation of our model.

Numeric Results

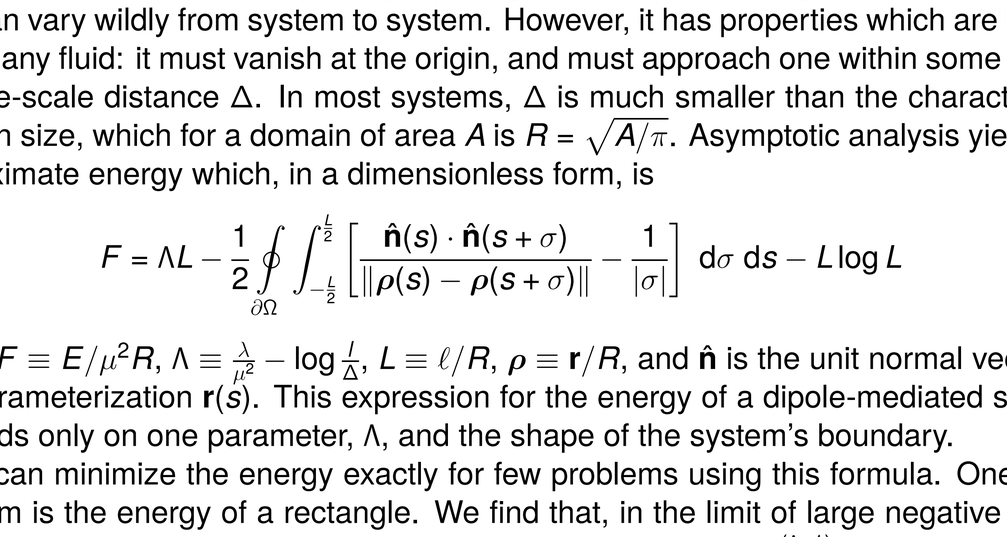

Figure 2: Harmonic bifurcations from the circular domain. Solid and dashed lines denote stable and unstable branches, respectively. The dots denote the theoretical bifurcation points.

We built a library for minimizing the function F using a modified Levenberg—Marquardt algorithm. With that system, we resolved the harmonic bifurcation of domains from a circle, including subcritical branches (see Fig. 2). Under ordinary circumstances we only found three nontrivial energy minimizers: the stripe (an elongated dogbone), forked, and doubly forked domains (see Fig. 3). In order to generate more realistic structures, we added a random energy background to F. This background consists of a sum of random sinusoids with total characteristic amplitude a_0. The result of this modification can be seen in Fig. 4, where domains at a variety of Λ and a_0 are shown.

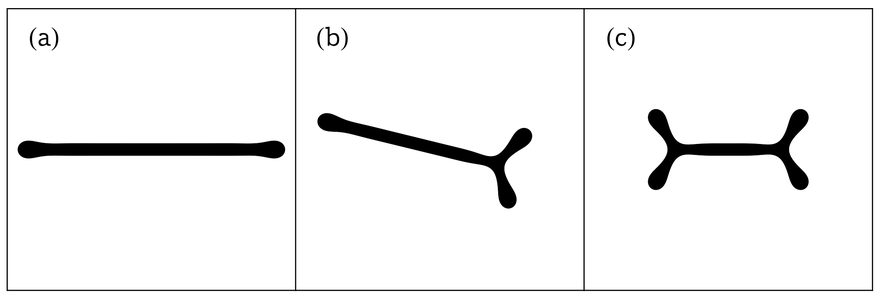

Figure 3: Representatives of (a) stripe, (b) forked, and (c) doubly forked domain morphologies at $\Lambda = -2$. These are the only stable morphologies in the absence of a random energy backdrop.

Finally we developed a simple model for extracting Λ. If a domain has a morphology with n junctions, then we reason that its perimeter should be approximately $L \simeq L_{\text{rec}} + (c+mn)w_{\text{rec}}$, where c and m are numeric constants. We use the three stable shapes in Fig. 3 to numerically solve for those constants. We can use this formula to solve for Λ, yielding

$$\Lambda' = \log\left[\frac{L-\sqrt{L^2-8\pi(c+mn)}}{2(c+mn)}\right] - 1$$

where Λ' denotes the value of Λ predicted by this model. The error of this analysis for samples of 50 domains generated at each Λ and a variety of random backgrounds can be seen in Fig. 5. Notice that while there are systematic differences between our model and the generating value Λ, the model consistently predicts Λ with less than 0.5% error.

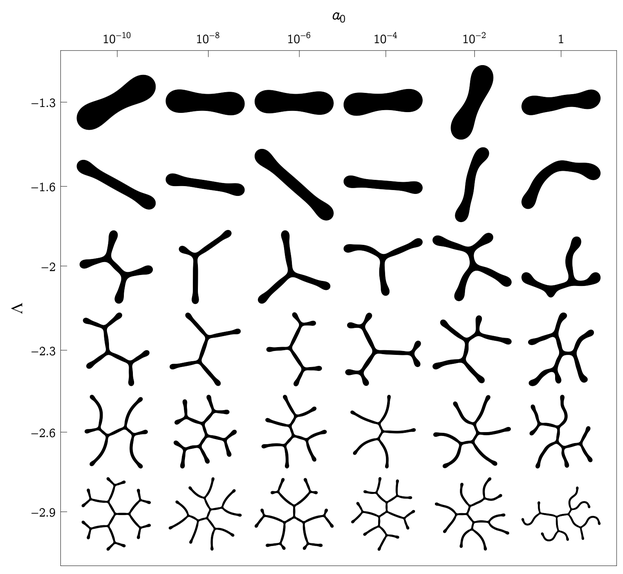

Figure 4: A sampling of stable domains generated over a random energy background. Moving along the x axis corresponds to changing a_0, the average magnitude of the background, and moving along the y axis changes Λ. All domains shown here are simulated with 1200-point boundaries.

Conclusions

We have created a general energy formulation of dipole-mediated systems and used it to numerically find stable domain structures. Adding a random energy background recovers the qualitative features of experimental domains. With these tools, we found a simple model which allows one to extract the parameter Λ from a domain structure using only its perimeter and the number of junctions it contains. We are currently working on producing a more accurate numeric analysis of our model for extracting Λ, and are also exploring options for the experimental verification of our model

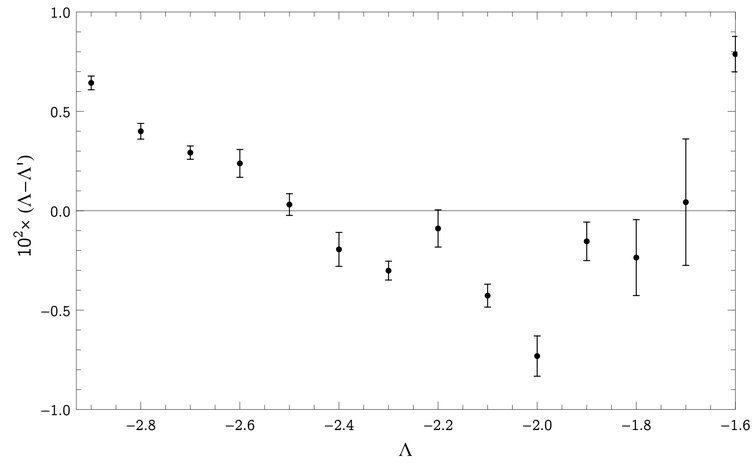

Figure 5: The difference between the generating value Λ and the mean predicted value Λ' for domains with 1200-point boundaries. The error bars denote standard error.

Acknowledgements

We would like to thank Chad Higdon-Topaz of Macalester College and the NSF (grant DMS-1009633) for supporting our research during the summer of 2013. We would also like to thank the Mathematics and Biology departments of Harvey Mudd College for use of their computing facilities.

Further Information

The senior thesis project which contains the work described here (and more) can be found online at `http://kent-dobias.com/kent-dobias_thesis.pdf`. The entirety of the code used in the numerics for this project is released under the GPL and can be found online at `https://github.com/kentdobias/dipole`. This poster is online at `http://kent-dobias.com/kent-dobias_thesis_poster.pdf`. Comments and questions about this work should be directed to `jkentdobias@hmc.edu`.