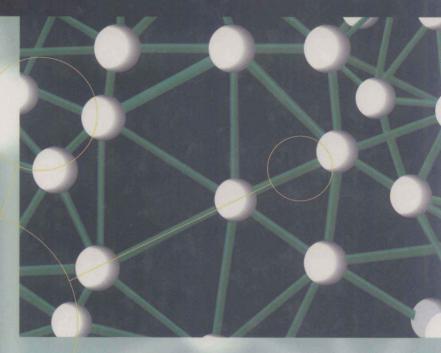
Defects and Geometry in Condensed Matter Physics



David R. Nelson

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Defects and Geometry in Condensed Matter Physics

This book describes the key role played by thermally excited defects such as vortices, disclinations, dislocations, vacancies and interstitials in the physics of crystals, superfluids, superconductors, liquid crystals and polymer arrays.

Geometrical aspects of statistical mechanics become particularly important when thermal fluctuations entangle or crumple extended line-like or surface-like objects in three dimensions. In the case of entangled vortices above the first-order flux lattice melting transition in high-temperature superconductors, the lines themselves are defects. A variety of theories combined with renormalization-group ideas are used to describe the delicate interplay among defects, statistical mechanics and geometry characteristic of these problems in condensed matter physics.

This indispensible guide has its origins in Professor Nelson's contributions to summer schools, conference proceedings and workshops over the past twenty years. It provides a coherent and pedagogic graduate-level introduction to the field of defects and geometry.

DAVID NELSON is Mallinckrodt Professor of Physics and Professor of Applied Physics at Harvard University. He received his Ph.D. in 1975 from Cornell University. His research focuses on collective effects in the physics of condensed matter, particularly on the connections between thermal fluctuations, geometry and statistical physics. In collaboration with his Harvard colleague, Bertrand I. Halperin, he has proposed a theory of dislocation- and disclination-mediated melting in two dimensions. Professor Nelson's other interests include the statistical mechanics of metallic glasses, the physics of polymerized membranes, vortex phases in high-temperature superconductors and biophysics.

Professor Nelson is a member of the National Academy of Sciences, a member of the American Academy of Arts and Sciences and a Fellow of the American Physical Society; he has been an A. P. Sloan Fellow, a Guggenheim Fellow and a Junior and Senior Fellow in the Harvard Society of Fellows. He is the recipient of a five-year MacArthur Prize Fellowship, the National Academy of Sciences Prize for Initiatives in Research and the Harvard Ledlie Prize.

To Patricia, Meredith, Christopher and Peter

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Preface to the book

Considerable relief accompanies completion of a project like this, especially one pursued (intermittently) for a period of eighteen years! There are many people to thank, not the least of which are the numerous graduate students, postdocs and other colleagues mentioned in Chapter 1 and in the acknowledgements of the remaining chapters. However, I owe a special debt to Michael Fisher, Leo Kadanoff and Bert Halperin, who provided inspiring examples of how to do theoretical physics early in my career. I am also grateful to Harvard University and the National Science Foundation of the USA, for creating the environment and freedom to do curiosity-driven research for the past twenty-five years.

I was fortunate to find a sympathetic publisher in Cambridge University Press. Simon Capelin and Rufus Neal provided expert editorial guidance and extraordinary patience in face of distractions caused by, among other things, my three years as Chair of the Harvard Physics Department. The original documents on which the last eight chapters are based illustrate the recent history of scientific publishing. At least one chapter evolved from an old-fashioned typewritten manuscript. Others originally appeared via a photographic offset printing process. The later chapters were created using LaTex and at least one is available (in an early form) on the World Wide Web (http://arXiv.org/abs/condmat/9502114). I appreciate the willingness of the original publishers to allow me to adapt my contributions to various proceedings, summer schools and workshops. I owe a special debt to Sally Thomas, Steven Holt, Jo Clegg and Jayne Aldhouse for the expert way in which they created a seamless high-quality book from these disparate media. Saul Teukolsky, Paul Horowitz and Renate D'Archangelo kindly provided advice and assistance with the index.

Farid Abraham generously assisted with the preparation of the illustration on the front cover. For more beautiful images created by Farid and his collaborators, see his gallery (http://www.almaden.ibm.com/vis/membrane/gallery.html). The pictures on the back cover are double-sided decorations of flux lines in high-temperature superconductors, due to Zhen Yao, Charles Lieber and their associates. I am grateful to Zhen and Charlie for permission to use their remarkable images, which

led to the first experimental measurement of a bosonic "phonon-roton" spectrum for entangled vortex lines. For a more detailed discussion, see the article with George Crabtree in the April 1997 issue of *Physics Today* and references therein. While going over the final page proofs, I was struck again by the many striking and experimentally observable manifestations of geometry, defects and statistical mechanics in condensed-matter physics. I hope others will be able to capture some of this excitement while reading this book.

David R. Nelson Rhinelander, Wisconsin September, 2001

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Chapter 1

Fluctuations, renormalization and universality

The idea of a book on defects and geometry in condensed matter physics slowly nucleated as I prepared contributions to various reviews, schools and workshops during the period 1982 to 1996. Although I have other interests in theoretical physics, I kept coming back at regular intervals to the statistical mechanics of defects and to related problems in the physics of flexible lines and surfaces. A consistent picture of these phenomena began to emerge and it transpired that work published in various forums during the early 1990s built on research I had described, e.g., at a summer school in the 1980s. Because considerable time and effort went into these reviews and all areas described are still active fields of investigation, it seemed reasonable to combine eight of them with this new introductory chapter in book form. The result, I hope, is a reasonably coherent account of the fascinating interplay among defects, geometry and statistical mechanics which has played such a central role in condensed matter physics during the past quarter century [1].

All chapters emphasize research in which I had a direct role. I have not attempted exhaustive reviews of these subjects and I apologize in advance to those whose work I have overlooked or neglected. These chapters are aimed at graduate students in physics, physical chemistry and chemical engineering as well as at more advanced researchers. Whenever possible, I tried to make the material intelligible to experimenters as well as theorists and to mention the many ingenious experiments which motivate the theories.

Condensed matter theorists owe a tremendous debt to our friends in the experimental community. They challenge us to *predict* and not

merely *postdict* experimental phenomena. Our experimental colleagues will go to great lengths to design an experiment capable of testing an interesting new theoretical idea. Theorists must be careful what they say, because predictions in condensed matter physics can often be tested in a matter of months with relatively inexpensive table-top experiments. We owe our colleagues in the laboratory a great debt because they keep us honest and inspire us with their beautiful experiments.

I also owe a special personal debt to the numerous theoretical graduate students, postdoctoral fellows and scientific colleagues who have contributed to the ideas in this book. Without their enthusiasm, dedication and many crucial insights this work would not have been possible.

This book describes, among other things, the statistical mechanics of vortices, disclinations, dislocations, vacancies and interstitials. Excitation of these defects in crystals, superfluids, superconductors, liquid crystals and polymer arrays usually requires strong thermal fluctuations. Geometrical aspects of statistical mechanics, with or without defects, often become particularly interesting when these fluctuations entangle or crumple extended line-like or surface-like objects in three dimensions. Sometimes, as is the case for entangled vortices above the first-order flux lattice melting transition in type-II superconductors, the lines themselves are defects! Because modern ideas about the renormalization group and universality in the presence of fluctuations underpin most of the work on defects and the statistical mechanics of lines and surfaces in this book, the remainder of this chapter provides a brief introduction to this point of view with several illustrative examples. We conclude with a survey of subsequent chapters.

1.1 Fluctuations and universality in condensed matter physics

Condensed matter physics flourished in the second half of the twentieth century, due in part to the application of sophisticated tools for understanding thermal and quantum fluctuations to an astonishing variety of problems. The failure of uncontrolled "mean field" or decoupling approximations is particularly evident close to equilibrium critical points, where fluctuations occur over multiple length scales, from an atomic dimension of order ångström units to a (diverging) correlation length which can be micrometers or more. The renormalization group, which was exported from particle physics by Kenneth Wilson in the early 1970s, allows a systematic understanding of such nested length scales (see Appendix A for an elementary introduction to the renormalization group in the "hydrodynamic" context considered here). A particularly striking result is that most of the detailed physics of matter at

microscopic length scales is *irrelevant* for critical-point phenomena. One can make precise quantitative predictions about certain "universal" critical exponents or scaling functions without getting the microscopic physics right in detail. What matters is symmetry, conservation laws, the range of interactions and the dimensionality of space. The physics of the diverging fluctuations at a critical point on large length scales is largely decoupled from the physics on atomic scales of order ångströms. The idea of new universal laws of physics governing fluctuations at a critical point was nicely summarized by A. Z. Patashinskii and V. L. Pokrovskii [2], two pioneers of scaling ideas at critical points in the USSR, who wrote that

When fluctuations, these shapeless amoebas, overlap in large numbers to form a continuous, undescribable soup, new and sharply defined laws . . . come into play, cutting through the chaos.

It turns out that not just critical points but entire phases of matter are described by a "universal," coarse-grained, long-wavelength theory. This point was recognized by Wilson [3], who argued that Landau's hydrodynamic treatment of magnets far from critical points (carried out in the 1930s) was itself representative of a particularly simple renormalization group fixed point. One can make similar statements about the hydrodynamic laws derived for fluids in the nineteenth century. Upon systematically integrating out the high-frequency, short-wavelength modes associated with atoms and molecules, one should be able to arrive at, say, the Navier-Stokes equations. One does not have to be at a critical point to have universal physical laws insensitive to the microscopic details. We now have many concrete calculations well away from critical points that support this point of view. Ignorance about microscopic details is typically packaged into a few phenomenological parameters characterizing the "fixed point," such as the density and viscosity of an incompressible fluid like water in the case of the Navier-Stokes equations.

The modern theory of critical phenomena has interesting implications for our understanding of what constitutes "fundamental" physics. For many important problems, a fundamental understanding of the physics involved does *not* necessarily lie in the science of the smallest available time or length scale. The extreme insensitivity of the hydrodyamics of fluids to the precise physics at high frequencies and short distances is highlighted when we remember that the Navier–Stokes equations were derived in the early nineteenth century, at a time when even the discrete atomistic nature of matter was in doubt. The same equations would have resulted had matter been continuous at all length

scales. The existence of atoms and molecules is irrelevant to the profound (some might even say "fundamental") problems of understanding, say, turbulence in the Navier–Stokes equations at high Reynolds numbers [4]. We would face almost identical problems in constructing a theory of turbulence if quantum mechanics did not exist, or if the discreteness of matter first became noticeable at length scales of order fermis instead of ångström units.

Many aspects of condensed matter physics, by which I mean the study of matter at everyday length and energy scales, do, of course, depend crucially on quantum mechanics and the particulate nature of matter. We cannot begin to understand phonons in solids, the specific heat of metals, localization in semiconductors, the quantum Hall effect and high-temperature superconductivity without knowing about the quantum mechanics of protons, neutrons, electrons and, occasionally, muons and positrons. There comes a point, however, when a more traditional reductionist approach burrows down to such short length scales and high energies that its conclusions become largely irrelevant to the physics of the world around us. This is why most condensed matter physicists are not aiming to discover the "fundamental" laws at the smallest length scales. The reductionist school of high-energy physics continues to be a noble intellectual enterprise, but is now virtually decoupled from physics at angström-unit scales, just as atomic physics is decoupled from the Navier-Stokes equations. New particles discovered in high-energy physics are unlikely to help us understand problems like turbulence or how itinerant magnetism arises from the Hubbard model; neither will they unravel other hard problems like the complexities of reptation dynamics in entangled polymer melts [5].

Although the precise nature of physics at very short length scales need not have a profound impact on deep unresolved questions at much larger scales, knowledge of the correct short-distance theory is of course far from useless in condensed matter physics. A first-principles calculation of the viscosity and density of water, for example, would require a molecular or atomic starting point. Deriving hydrodynamic parameters such as the viscosity from an atomistic framework is the task of kinetic theory, in which significant progress has been made during the last century, at least for weakly interacting gases; and we are impressed when *ab initio* band-structure experts are able to correctly predict the lattice constant and crystal structure of silicon via numerical solutions of Schrödinger's equation. Nevertheless, there will always be important problems that a strict *ab initio* approach based on a more fundamental theory are unlikely to resolve.

The problems discussed in this book are all represented by coarsegrained long-wavelength "hydrodynamic" models, with the detailed physics packaged into a small number of phenomenological coupling constants. To illustrate the approach, we discuss two interesting but unusual situations in which ratios of long-wavelength hydrodynamic parameters are themselves universal constants, just like the universal exponents at a critical point. The first is the universal value of the Prandtl number of a two-dimensional incompressible fluid (it equals $(\sqrt{17}-1)/2)$ and the second is the universal (negative!) value of Poisson's ratio associated with polymerized membranes or "tethered surfaces" (it is about $-\frac{1}{3}$). We then review the role of topological defects in destabilizing the hydrodynamic surface of fixed points associated with two-dimensional crystals. Here, the physics associated with strong thermal disorder leads to models dominated by fluctuations in the phase of the translational and orientational order parameters, instead of the usual amplitude fluctuations associated with mean field or Landau theories. Amplitude fluctuations now reside only in the cores of defects such as dislocations and disclinations. We discuss the new fixed point that takes over in membranes characterized by a bending rigidity, where defects such as dislocations can buckle easily out of the plane. This introduction concludes with an overview of the contents of the rest of the book

1.2 The universal Prandtl number in two-dimensional hydrodynamics

Understanding chaotic fluid flows, particularly those at high Reynolds numbers, remains one of the most challenging problems in theoretical physics and fluid mechanics, despite the concerted efforts of many experts during the past half century [4]. Under many circumstances, it is expected that the fluid velocity field $\mathbf{v}(\mathbf{r}, t)$ and the concentration $\psi(\mathbf{r}, t)$ of tracer particles are described by the equations

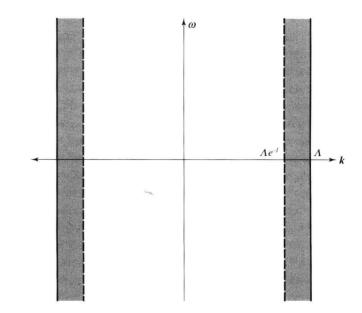
$$\partial_t \mathbf{v} + (\mathbf{v} \cdot \nabla) \mathbf{v} = -\frac{1}{\rho} \nabla p + \nu \nabla^2 \mathbf{v}, \tag{1.1}$$

$$\nabla \cdot \mathbf{v} = 0, \tag{1.2}$$

$$\partial_{t}\psi + (\mathbf{v}\cdot\nabla)\psi = D\nabla^{2}\psi,\tag{1.3}$$

where ν is the kinematic viscosity, ρ is the density of the fluid, D is the diffusivity of the tracer particles and the condition of incompressibility (which is valid in the limit of velocities much less than the speed of sound) is enforced by Eq. (1.2). This condition can be used to eliminate the term involving the pressure field, $p(\mathbf{r}, t)$, in Eq. (1.1). The dynamics becomes insensitive to the density. Equations (1.1)–(1.3) then represent a "universal" long-wavelength, low-frequency description of a large number of atomic and molecular fluids, parameterized only by the

Fig. 1.1. The degrees of freedom for a randomly stirred Navier-Stokes fluid. indexed by wavevector and frequency, with wavevectors above a cutoff Λ excluded. A renormalization group transformation focusing on the long-wavelength hydrodynamic behavior can be constructed by iterative elimination of Fourier modes in a shell of wavevectors in the range $\Lambda \exp(-\ell) < k < \Lambda$ indicated by the shaded region.



viscosity ν and the diffusivity D. If a colored dye of tracer particles is injected into water, one has $\nu \approx 10^{-2}$ cm² s⁻¹ for the viscosity and $D \approx 10^{-6}$ cm² s⁻¹ for the molecular diffusivity and thus the dimensionless "Prandtl number" is

$$Pr = \nu/D \approx 10^4. \tag{1.4}$$

However, in general, one would expect that the Prandtl number could assume any positive value in a three-dimensional fluid. This is not the case in two dimensions!

By including various additive forcing terms on the right-hand side of Eqs. (1.1) and (1.3), one can simulate the effects of thermal fluctuations or even random stirring which can provoke chaos and high-Reynolds-number turbulence. The influence of the nonlinear terms $((\mathbf{v} \cdot \nabla)\mathbf{v})$ and $(\mathbf{v} \cdot \nabla)\psi$ on the physics at long wavelengths can be assessed by the iterative coarse-graining procedure embodied in the renormalization group. The idea behind this perturbative renormalization procedure is reviewed in Fig. 1.1 [6, 7]. The velocity field of a *d*-dimensional fluid is first decomposed into Fourier modes according to

$$\mathbf{v}(\mathbf{r}, t) = \int_{k < \Lambda} \frac{d^d k}{(2\pi)^d} \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \mathbf{v}(\mathbf{k}, \omega) e^{i\mathbf{k}\cdot\mathbf{r} - i\omega t}.$$
 (1.5)

The spatial modes are cut off above a spatial wavevector $k=\Lambda$ of order the inverse interparticle separation and the frequencies are unconstrained. The equations of motion for modes in the range $\Lambda/e^{\ell} < k < \Lambda$ are formally solved (via a diagrammatic perturbation theory) and these solutions then substituted into the equations of motion for the remaining