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Discrete Energy on Rectifiable Sets

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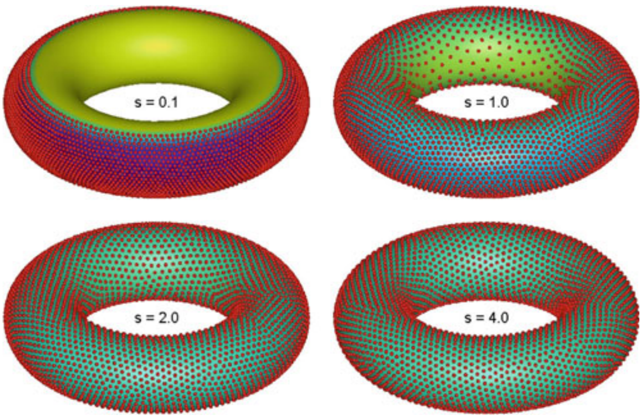

Equilibrium configurations for four different interacting systems of 4000 particles restricted to the surface of an embedded torus. Interactions are of the form $1/r^s$, where r is the distance between points and $s = 0.1, 1, 2$, and 4, illustrating the Poppy-seed bagel theorem (Theorem 8.5.2)

To our wives,

Viktoriia Malakhova
Anne Hardin
Loretta Saff,

who have added true equilibrium
to our lives.

Preface

Our goal is to provide an introduction to the study of minimal energy problems, particularly from the perspective of generating point configurations that provide useful discretizations of manifolds. In so doing, we hope to convey the beauty of the subject and to emphasize its connections with various branches of mathematics such as potential theory, geometry, numerical analysis, graph theory, coding theory, among others. And, although not specifically addressed in these pages, we wish to emphasize that such energy problems arise in a myriad of optimization problems of relevance to the physical, chemical, and biological sciences.

In its most general form, the discrete energy problems we consider are those that arise from pairwise interactions as follows. Given a compact set A in Euclidean space, a lower semicontinuous kernel $K(\cdot,\cdot)$ $A \times A \to \mathbb{R} \cup \{+\infty\}$, and an integer $N \geq 2$, assign to every N-point subset ω_N of A its K-energy

$$E_K(\omega_N) := \sum_{\substack{x \neq y \\ x,y \in \omega_N}} K(x,y),$$

and seek a configuration ω_N^* that minimizes this energy. Such problems can be viewed as generalizations of Thomson's classic "plum-pudding" model for the atom, where A is the unit sphere in $\mathbb{R}^3$ and $K(x,y) = 1/|x-y|$ simulates the interaction between electrons. The reciprocal distance kernel (or Coulomb potential) belongs to the class of Riesz s-kernels defined by $K_s(x,y) = 1/|x-y|^s$, a class to which we pay particular attention. One of our goals is to explore the global and local properties of minimizing configurations as the parameter s varies. Cases for which K_s is integrable with respect to some finite product measure $\mu \times \mu$ on $A \times A$ fall under the umbrella of classical potential theory for which we provide a synopsis in Chapter 4. A somewhat unique feature of the book is the exploration (beginning with Chapter 8) of minimizing configurations for non-integrable Riesz kernels (typically when $s \geq \dim A$). In physics terminology, we analyze the asymptotic behavior of minimizing (and close to minimizing) N-point configurations as $N \to \infty$ for both "long-range" and "short-range" interactions as well as for the critical parameter $s = \dim A$ at which the transition takes place. While a major component of this work deals with "large N" results we also consider some very special finite problems for which explicit solutions are known.

Point configurations on the sphere are of wide interest and they are addressed throughout the book. Moreover we specifically devote Chapters 5, 6, and 7 to this topic that includes the universal optimality theory of Cohn and Kumar as well as a comparison of several "popular methods" for uniformly distributing points on the two-dimensional sphere, which we hope will serve as a convenient resource. Other noteworthy features of the book include chapters on best-covering and best-packing (Chapters 3 and 13), an analysis of periodic energy problems for "Gauss-type" potentials generated by signed measures (Chapter 10), and a treatment of optimal discrete measures for potentials (which we call polarization or Chebyshev problems) in Chapter 14. These chapters include a number of previously unpublished results. Rather than delving more deeply here into the contents and underpinnings of the book, we provide a brief "Overview" chapter (Chapter 0) that serves as a more detailed prospectus.

Because the subject of minimal energy is broad and dynamic, we have been forced to make difficult decisions regarding the length and breadth of our treatment. Indeed, new and significant results are appearing regularly in the literature making a completely thorough and up-to-date compilation of all known results on the subject beyond our means. We also regret not providing in-depth discussions of the proofs of some significant results such as the best-packing densities in dimensions 3, 8, and 24, as these results require considerably more background and exposition than the limitations of length for an introductory book would allow. And we further apologize that little attention is given to topics such as the random generation of point configurations and their local properties. Nonetheless, it is our hope that this opus serves as a useful introduction to minimal energy problems—one that inspires further exploration of the subject and its multitude of connections to the mathematical sciences.

We have endeavored to give well-deserved acknowledgments to those researchers whose results are quoted in the book, but it is inevitable that there are unintended oversights for which we apologize in advance. Our hope is that the reader will call such omissions to the attention of the authors so that we might correct them in a future printing. Citations to the literature are mainly reserved for the Notes and Historical References sections that appear at the end of each chapter. In so doing we minimize interruption to the exposition. Also in these closing sections, the reader will find discussions of alternative proofs or related topics.

We have written the book with graduate students in mind. What is required of the reader is essentially a year-long graduate course in Real Analysis, which we augment and reinforce with a chapter entitled Preliminaries (Chapter 1), where we discuss topics such as Hausdorff measure, weak-star convergence of measures, the Fourier transform, and Poisson summation. In addition, several topics not covered in detail in the main part of the book are treated in the Appendix, such as completely monotone functions and properties of orthogonal polynomials. In this way, we have striven to make the book mostly self-contained.

We are indebted to a large cast of students and distinguished colleagues, who have provided us with valuable input on the manuscript. Our gratitude goes, especially, to R. Womersley for his computations and illustrations that adorn many pages of the book. To the Vanderbilt team of T. Michaels, A. Reznikov, and O. Vlasiuk, who met regularly to provide us with useful feedback on the book, we express our sincere appreciation. We also wish to acknowledge very helpful suggestions from J. Brauchart, P. Dragnev, D. Ferizovic, P. Grabner, W. Kusner, V. Maymeskul, B. Simanek, and C. Villalobos Guillen.

Our research relating to the topics of this book has spanned many years during which time the National Science Foundation of the U.S.A. has provided crucial support. We are truly appreciative of NSF's recognition of our work.

Several phases of the writing of this book and related research articles were conducted at the Mathematics Research Institute in Oberwolfach (MFO), Germany, and at the Institute for Computational and Experimental Research in Mathematics (ICERM) at Brown University, Providence, RI. We are grateful to the administrations of the MFO and ICERM for providing us with such stimulating and pleasant environments. Finally, we want to thank the staff at Springer, particularly Elizabeth Loew, for her encouragement, patience, and persistence in bringing this work to fruition.

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Contents