STATEMENT OF RESEARCH

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As an undergraduate I enjoyed studying analysis and knew that I wanted to work in a related field for my dissertation. My dissertation research concerns complex analytic, functional analytic, and representation theoretic methods applied to the two-dimensional periodic Ising model which is a model in statistical mechanics. I have published two papers related to the Ising model [11], [19]. During my postgraduate years, I found that I was drawn to analysis and statistics applied to real world problems. Currently, my research focus has been on solving statistical problems in the new field of Mineral Evolution. This work is a result of an interdisciplinary collaboration effort between a group of geoscientists at the University of Arizona and the Carnegie Institution of Washington.

I will introduce the Ising model and provide related results in section 1 and 2 followed by a discussion of potential research problems in section 3. The statistics of Mineral Evolution will be described in section 4 followed by a discussion of plans for future research in section 5. In this section, we also describe a pending grant proposal as well as potential research projects for undergraduates. Authored and coauthored papers related to this work are given in [6], [7], [8], [9], [12], and [13].

1. Introduction to the periodic Ising model

The Ising model is one of the most studied models in modern physics. Since its introduction in 1925 by E. Ising, more than a thousand research papers have been published on the subject. The model has had great success in shedding light on the existence of phase transitions at a finite temperature T_C (critical temperature). The simplicity of the model made it possible to obtain exact mathematical results in the thermodynamic limit of statistical mechanics.

The model lives on a finite $(2M+1)$ by $(2N+1)$ lattice, where M and N are positive integers. Each vertex is assigned a spin value of $+1$ (spin up) or -1 (spin down). A configuration σ is a particular assignment of spin values to the vertices, in which the value at a site is a ±1-valued random variable. We are interested in the case where σ satisfies periodic boundary conditions. The interaction energy, $E_{M,N}$, of a periodic configuration in the absence of an external magnetic field is computed by summing over all nearest-neighbors spins. The partition function, $Z_{M,N}$, is the sum of Boltzmann weights for a configuration. The probabilistic information in the model is given in terms of the *correlation functions* defined as the expected values of products of spin variables at sites $j_1, ..., j_k$,

$$\langle \sigma_{j_1} \cdots \sigma_{j_k} \rangle_{M,N} = \frac{1}{Z_{M,N}} \sum_{\sigma} \sigma_{j_1} \cdots \sigma_{j_k} \exp\left(- \frac{E_{M,N}(\sigma)}{k_B T} \right),$$

where T is the temperature and k_B is the Boltzmann constant. Kaufman [15] showed that the partition function can be written as the trace of the $2N+1$ power of a transfer matrix, V, that can be characterized as an element in a spin representation of the orthogonal group,

$$Z_{M,N} = \mathrm{Tr}(V^{2N+1}).$$

Using this representation of the transfer matrix, Kaufman [15] determined its spectrum on the finite periodic lattice, and her derivation was a simplification of Onsager's [17] famous result on solving the two-dimensional Ising Model. Onsager computed the exact value of the specific heat as a function of temperature in the thermodynamic limit by showing that the partition function can be approximated by the largest eigenvalue of the transfer matrix.

2. Results regarding the Ising model

My main concern in [11] was the calculation of the matrix representation of the spin operator on the finite periodic lattice in an orthonormal basis of eigenvectors for the transfer matrix. These spin matrix elements have consequences for the computation of all multi-point Ising Correlation functions on the cylinder and torus. In 2003, Bugrij and Lisovyy [2], [3] proposed explicit formulas for such elements, but the proof of the conjecture, given in [20] and [21], was extremely complicated. My paper aimed toward constructing a simple proof even though there were a few technical difficulties that remained to be resolved. In [11], I first reworked Kaufman's famous 1949 paper [15] on the periodic Ising model by using representation theory. My approach provided a new feature which led to a simpler and more direct way of computing the spectrum of the transfer matrix. Some details of this approach will be described next.

For periodic boundary conditions on the lattice, the $2M+1^{th}$ roots of unity, $z^{2M+1} = 1$, are relevant as are the $2M+1^{th}$ roots of -1, $z^{2M+1} = -1$. I will refer to these two finite sets as the periodic spectrum Σ_P and the anti-periodic spectrum Σ_A. Define the parity operator $U = \prod_{k=-M}^{M} ip_k q_k$, where $\{q_k, p_k\}$ are certain representations of the Clifford relations, and also a basis for the finite sequence space, $W := l^2(-M, ..., M, \mathbb{C}^2)$. Let $(U = \pm 1)$ denote the ± 1 eigenspaces of U. Kaufman [15] showed that the transfer matrix V can be written as the direct sum $V = V^A \oplus V^P$, where $V^A = V|_{(U=1)}$ and $V^P = V|_{(U=-1)}$. The letters A and P refer to the restriction to the anti-periodic and periodic spectrum respectively. Let $T^A(V)$ denote the induced rotation in the anti-periodic Fourier representation associated with V^A with a completely analogous definition for $T^P(V)$. The induced rotation associated with V is a complex orthogonal matrix which completely determines the transfer matrix. Both T^A and T^P have positive real spectrum that does not contain 1. I am interested in the two isotropic splittings,

$$W = W_+^A \oplus W_-^A \quad \text{and} \quad W = W_+^P \oplus W_-^P,$$

where W_+^A denotes the span of the eigenvectors for $T^A(V)$ associated with the eigenvalues between 0 and 1, and W_-^A denotes the span of the eigenvectors for $T^A(V)$ associated with the eigenvalues greater than 1. Let T_+^A denote the restriction of $T^A(V)$ to W_+^A. The subspaces $W_\pm^P$ and the operator T_+^P are defined in an analogous way. A principal result I derived in [11] is that the eigenspace $(U = 1)$ is unitarily equivalent to the even tensor algebra over W_+^A, and $(U = -1)$ is unitarily equivalent to the even tensor algebra over W_+^P. In this representation, there is an explicit model for V^A and V^P where the vacuum vector is an eigenvector associated with the largest eigenvalue of the transfer matrix.

By using this result, I determined in [11] formulas for the spin matrix elements that depend on the matrix elements of the induced rotation associated with the spin operator in a basis of eigenvectors for the transfer matrix. The representation of the spin matrix elements was obtained by regarding the spin operator as an intertwining map for the periodic and anti-periodic Fock representations,

$$\sigma : \mathrm{Alt}_{\mathrm{even}}(W_+^P) \to \mathrm{Alt}_{\mathrm{even}}(W_+^A).$$

The induced rotation, $T(\sigma)$, for the spin operator is the identity on W. Suppose

$$\begin{pmatrix} A & B \\ C & D \end{pmatrix}$$

is the matrix of this map on W going from the $W_+^P \oplus W_-^P$ splitting to the $W_+^A \oplus W_-^A$ splitting. I was interested in finding the inverse of D, where D is invertible when the one-point function is nonzero. By using a Berezin integral representation [4] for the matrix elements of the Fock representation of an element in the Clifford group, I have in [11] provided formulas for the spin matrix elements that depend on the inverse, D^{-1}. In particular, I showed that the simplest spin matrix elements, i.e. the two-point functions, can be written in terms of D^{-1}, BD^{-1} and $D^{-1}C$. It is an extremely difficult task to invert D, and in [11] I only had a formula for it in terms of a Bugrij-Lisovyy conjecture [2], [3] for the spin matrix elements on the finite periodic lattice. I showed that the spin matrix elements can be written as Pfaffians of skew symmetric matrices whose elements are multiples of the two-point functions. By using the proposed Bugrij-Lisovyy formulas for these elements combined with an elliptic substitution of the spectral curve, I showed that the conjecture for the two-point functions leads to the general formula.

In the paper [19], we applied the technique in [16] to compute the matrix representation for the spin operator in a basis of eigenvectors for the transfer matrix in the scaling limit of the periodic Ising model. The technique we used was to single out an appropriate Green function for the Dirac operator on the cylinder in the continuum that connects to the scaling limit calculations of D^{-1}. The spin matrix representation given in [19] leads to formulas for the correlations in the scaling limit for the cylinder and for the torus. We have not controlled the convergence of the scaling limit in the paper [19]. This convergence result is provided in my thesis [10] assuming the Bugrij-Lisovyy conjecture. There I regarded the correlations as vacuum expectations of products of spin operators in the scaling limit $n \to \infty$ of the cylinder, and given in terms of the Bugrij-Lisovyy conjecture for the spin matrix elements on the finite periodic lattice.

3. POTENTIAL RESEARCH REGARDING THE ISING MODEL

In 2011, N. Iorgov and O. O. Lisovyy [14] proved the eight year old Bugrij-Lisovvy conjecture based on the results of our papers [11] and [19]. They were able to find a formula for the inverse D^{-1}. We then now have explicit formulas for the spin matrix elements on the finite periodic lattice which is equivalent to the computation of the multi-point spin correlation functions on the cylinder and torus. In the paper [19] we considered the scaling limit of the transfer matrix and the spin operator without attempting to control the convergence. The result for the convergence problem concerning the cylinder is given in my thesis [10] assuming the Bugrij-Lisovvy conjecture. Since the Bugrij-Lisovyy conjecture is now proved we can control the scaling limit of the correlation functions on the cylinder for the finite periodic Ising model as the temperature approaches the critical temperature from below. We could also work out such a result for the torus. Furthermore, it would be interesting to calculate the scaling limit of the correlation functions on the cylinder and torus for temperatures above the critical temperature. It will also be useful to find a meaningful way to compare the correlation functions on the periodic lattice with the correlation functions computed in the infinite-volume limit.

4. Statistical Analysis of Mineral diversity

The search for predictive statistical models of natural systems represents an ongoing opportunity and challenge in applied mathematics. We employed the extensive and growing data resources on mineral species and their localities to identify and parameterize frequency distributions of Earth's mineral kingdom. These models, for the first time, facilitate prediction of Earth's total, but as yet undiscovered, mineralogical diversity. We also demonstrated the high probability that no other planet or moon in the cosmos has the same mineralogical repertoire as Earth. We concluded that, in spite of deterministic chemical and biological factors that control most of our planet's mineral diversity, Earth is mineralogically unique in its distribution of rare species. The frequency distribution of mineral species in Earth's near-surface environment, as well as on other terrestrial planets and moons, arises from both deterministic factors and chance events [9]. We have identified predictive statistical models that describe the frequency distribution of mineral species on Earth. Discovering such models allows us to address questions such as:

- What is the number of distinct mineral species on Earth (i.e., how many mineral species are yet to be discovered)?
- If we were able to re-sample the mineral species on Earth with the same sample size and the same number of minerals were discovered anew, how many mineral species would differ from those known on Earth today?
- Could this distribution be used to characterize an "Earth-like" planet?
- Is Earth unique in terms of its mineralogy?

The mineral frequency distribution is a Large Number of Rare Event distribution (LNRE), where 34% of the approved mineral species are found at only one or two localities. Models from the family of LNRE distributions fit all mineral species as well as a subset consisting of only the mineral species that incorporate the rare element beryllium. We used simulation studies and techniques from the frequency distribution literature in the fields of ecology and linguistics [1], [5] which are also concerned with estimation of the sizes of type-rich populations. We found that at least 1500 mineral species remain to be discovered, employing current analytical techniques. Furthermore, a replay of mineral evolution on Earth, repeating the same deterministic factors, would result in more than 13.7% of mineral species different from those discovered thus far. We also found that the probability of an Earth-like planet, having the exact same mineral species as the observed beryllium mineral species on Earth is smaller than 1.4×10^{-10}.

5. Future work in statistical mineral evolution and grant proposal

The contribution [12] is the first in an anticipated series of studies that attempts to apply large mineralogical data resources and statistical methods to understand the diversity and distribution of mineral species on Earth, as well as other terrestrial planets and moons. Many avenues await further exploration. What model works best for other elements, or for subsets of mineral species-locality data that reflect geographic, age, tectonic, or other restrictive factors? Are any aspects of mineral frequency distributions indicative of life-biosignatures that might apply to other worlds? Do the simulation studies illuminate how to characterize an Earth-like planet? These questions will provide a dynamic focus for future studies.

Mineral Evolution is a new and open field with varied research potential spanning the search for ore resources and analysis of extraterrestrial planets. We have received a 1.3 million dollar research grant from the Keck Foundation over a 3 year period that started in 2015 and some start-up support from the Sloan Foundation and the Carnegie Institution of Washington. Currently, we have several undergraduates in geosciences working on collecting mineralogical data. There are several opportunities for an undergraduate in mathematics/statistics to conduct research in the statistical analysis of Mineral Evolution. While we have completed the statistical analysis for the beryllium mineral species, an undergraduate could analyze the rest of the elements by following the template that I created in the statistical software package R. This will engage an undergraduate doing applied research of unknown results while simultaneously learning the statistical methodologies.

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