Riemannian Geometry of Ising Model in the Bethe Approximation

Rıza Erdem
Department of Physics, Faculty of Science, Akdeniz University, Antalya, Turkey
E-mail: erdem@akdeniz.edu.tr

Abstract. A method combining statistical equilibrium theory and metric geometry is used to study thermodynamic scalar curvature in the neighborhood of the Curie critical temperature for an Ising model of ferromagnetism. Using a Bethe type free energy expression, a non-diagonal metric is introduced on the two-dimensional phase space of long-range and short-range order parameters. Based on the metric elements Christoffel symbols, curvature tensor and Ricci tensor are found. An expression (containing equilibrium order parameters) is derived for Riemann scalar curvature \( R \). Its behavior near the critical temperature is examined analytically. We find that \( R \) tends toward plus infinity while approaching the critical point. This result fits well with those in the exact one-dimensional chain and mean-field Ising model in the lowest order approximation.

1. Introduction
Ising model is a crude attempt to simulate the structure of a ferromagnetic substance. It has been thoroughly studied since its conception in the 1920’s [1] and hence become one of the most important models in modern physics. The dramatic rise in the level of mathematics used in examining the Ising model warrants much attention. Particularly, various authors motivated by ideas in the geometrical perspective on statistical mechanics, have drawn a geometrical structure for the Ising model using some space of parameters with a metric. For example, a Riemannian geometry (RG) has been introduced and applied to a number of Ising chains with exact solutions [2-8]. Moreover, the thermodynamic Riemann scalar curvature was examined for the same model under the approximate methods. In the application of the RG to Ising systems, nobody adopted the Bethe approximation because of its mathematical complexity, and restricted themselves to mean-field approximation, leading to new and alternative insights into physics of the magnetic phase transitions [2, 4, 7].

The present work focuses on the simple interpretation of the abrupt change in the geometrical properties in terms of that in static properties for the Ising system based on Bethe (or pair) approximation (an improvement over the mean-field approximation) near the transition temperature. This is achieved by the combination of statistical equilibrium theory and Riemannian metric geometry.

2. Model description and free energy in the Bethe approximation
The Ising model under study is an assembly of \( N \) spins localized on lattice points with properties that each spin can only be up (positive) or down (negative) direction along the \( z \)-axis and
spin-spin interactions are nearest-neighbor in range. Letting \( E, T \) and \( S \) be internal energy, temperature and entropy, respectively, the Helmholtz free energy (\( F = E - TS \)) of the system may be written in the Bethe approximation for given long range order \( x \) and short range order \( y \) as [9, 10]

\[
F(x, y) = -\frac{1}{2} N \gamma J y - g \mu_B H N x - kT \ln W(x, y),
\]

where \( \gamma, J, k, g, \mu_B, H \), are the number of nearest neighbors, the exchange integral (positive for ferromagnetism), Boltzmann constant, the spin factor, the Bohr magneton, and the external magnetic field, respectively. The third term in Eq. (1) is given by [10, 11]

\[
\ln W(x, y) = \frac{1}{2} N \left\{ \frac{2}{\gamma} \ln 2 + \left( 1 - \frac{2}{\gamma} \right) \left[ (1 + x) \ln(1 + x) + (1 - x) \ln(1 - x) \right] \right. \\
\left. - \frac{1}{2} (1 - y) \ln(1 - y) - \frac{1}{4} (1 + 2x + y) \ln(1 + 2x + y) - \frac{1}{4} (1 - 2x + y) \ln(1 - 2x + y) \right\}.
\]

In the absence of an external magnetic field \( H \), the equilibrium values of the long-range order and short range order, \( x_0 \) and \( y_0 \), respectively, are found from the conditions \( \frac{\partial F}{\partial x} = 0 \) and \( \frac{\partial F}{\partial y} = 0 \).

3. Basics of Riemannian geometry

We begin with a very brief overview of information geometry. A metric in equilibrium thermodynamic state space is defined by

\[
ds^2 = \sum_{i,j} g_{ij} d\theta^i d\theta^j,
\]

where \( \theta^i, i = 1, 2, ..., n \) denote various thermodynamic parameters. As shown by Ruppeiner [3], this metric introduces the concept of a distance in the space of equilibrium states. The curvature tensor may be written in terms of the metric elements \( g_{ij} \) as [3, 12]

\[
R_{ijkl} = \Gamma_{jk,i}^l - \Gamma_{jl,i}^k + \sum_{m=1}^n \Gamma_{jk}^m \Gamma_{im}^l - \sum_{m=1}^n \Gamma_{jl}^m \Gamma_{km}^i,
\]

where the Christoffel symbols are defined by

\[
\Gamma_{\nu\lambda}^\mu = \frac{1}{2} \sum_{\rho=1}^n g^{\mu\rho} \left( g_{\rho\nu,\lambda} + g_{\rho\lambda,\nu} - g_{\nu\lambda,\rho} \right).
\]

In Eq. (5), the comma notation \( (,) \) denotes the partial derivative with respect to the \( \mu \)th coordinate. The components of the second-rank Ricci tensor are

\[
R_{ij} = \sum_{m=1}^n R_{im}^m.
\]

Contracting the Ricci tensor yields the Riemannian scalar curvature

\[
R = \sum_{i,j=1}^n g^{ij} R_{ij}.
\]

The scalar curvature given by Eq. (7) measures the complexity of the system. Zero curvature corresponds to flat metric and a noninteracting physical system. When it is not zero (any positive or negative integer), the metric is not flat and the system is interacting. In this case, it plays a central role in any attempt to look at phase transitions from a geometrical perspective.
4. Derivation of Riemannian scalar curvature for the Ising model

For the Ising model in an external magnetic field we parametrize a two-dimensional Riemann manifold by \((\theta^i, \theta^j) = (x, y)\). In this case, the components of the metric take the simple form 
\[
g_{ij} = -\beta \partial_i \partial_j f
\]
where \(\beta = 1/kT\), \(\partial_i = \partial/\partial \theta^i\) and \(f = F/N\) (or the free energy per site) \[3\]. Using (3) we define the metric for the above spin system as
\[
ds^2 = g_{xx} dx^2 + 2g_{xy} dxdy + g_{yy} dy^2,
\]
and the components of the metric tensor \(g_{ij}\) is computed by means of Eqs. (1) and (2). According to the general rules developed above, we have
\[
g_{xx} = -\frac{1}{T} \frac{\partial^2 f}{\partial x^2} = -\gamma \left[ \frac{1 + y}{(1 + y)^2 - 4x^2} - \frac{1 - (1/\gamma)}{1 - x^2} \right],
\]
\[
g_{xy} = g_{yx} = -\frac{1}{T} \frac{\partial^2 f}{\partial x \partial y} = \gamma \frac{x}{(1 + y)^2 - 4x^2},
\]
\[
g_{yy} = -\frac{1}{T} \frac{\partial^2 f}{\partial y^2} = \gamma \frac{1 + y - 2x^2}{2(1 - y)} \left[ \frac{1 + y - 2x^2}{(1 + y)^2 - 4x^2} \right].
\]

With our metric tensor (9), due to Eqs. (4)-(7), after rather lengthy computations we have received the following simple expression for the scalar curvature \(R\) in terms of the known equilibrium quantities,
\[
R = \frac{AB}{C^2},
\]
with
\[
A = x_0^2 - 1,
\]
\[
B = -(\gamma - 2)x_0^2 + 2(\gamma - 1)y_0 - \gamma,
\]
\[
C = (\gamma - 2)x_0^2 - (\gamma - 1)y_0 + 1,
\]
where \(x_0\) and \(y_0\) are the equilibrium values of order parameters. These values can be written conveniently in terms of the Bethe long range order parameter \(\delta\) through the relations \[10, 11, 13\]
\[
x_0 = \tanh \gamma \delta,
\]
\[
y_0 = 1 - 2 \frac{\sinh(\gamma - 2)\delta}{\sinh(2\gamma - 2)\delta \cosh \gamma \delta},
\]
where the temperature dependence of \(\delta\) is given by
\[
\exp(-J/kT) = \frac{\sinh(\gamma - 2)\delta}{\sinh \gamma \delta},
\]
and the relation between \(\delta\) and the temperature slightly below the critical temperature \((T_c)\) is approximately written as \[10, 11\]
\[
\frac{2}{3}(\gamma - 1)\delta^2 = \frac{J \theta}{kT_c},
\]
where \(\theta = \frac{T - T_c}{T_c}\) is the distance from the critical temperature. In order to analytically examine scalar curvature (10) for temperatures just below \(T_c\), one may use the following series expansions for (12):
\[
x_0 = \gamma \delta - \frac{1}{3} \gamma^3 \delta^3 + \ldots,
\]
\[ y_0 = 1 - \left( \frac{\gamma - 2}{\gamma - 1} \right) \left[ 1 - \gamma \left( \frac{\gamma - 2}{3} \right) \delta^2 + \ldots \right]. \] (15)

Using (15), all the coefficients in (11) will be given in power series in \( \delta \) as follows

\[ A = -1 + \gamma^2 \delta^2 + \ldots, \]
\[ B = - (\gamma - 2) \left[ 1 - \gamma \left( \frac{1}{3} \right) \delta^2 + \ldots \right], \]
\[ C = \frac{2}{3} (\gamma - 2) \gamma \delta^2 \left[ 1 - \gamma^3 \delta^2 + \ldots \right]. \] (16)

Substituting Eqs. (16) into the expression (10) for scalar curvature near \( T_c \), one finally obtains

\[ R = \frac{9}{4 \gamma^2 (\gamma - 2) \delta^4} \left[ 1 + 2 \gamma \left( \gamma^2 - \gamma + \frac{2}{3} \right) \delta^2 + \ldots \right]. \] (17)

According to (17) we have two propositions for the critical behaviour of \( R \) as follows:

**Proposition 1.** When \( \gamma \) is a finite number, corresponding to a different lattice structure, \( R \) is always positive and tends to plus infinity \( (R \to \infty) \) near a non-zero critical temperature \( (\delta \to 0 \text{ or } T \to T_c) \) with only one exception, namely, that of linear chain \( (\gamma = 2) \). A one-dimensional Ising chain does not undergo a phase transition at a non-zero temperature. To test the behaviour of \( R \) for a lattice with \( \gamma = 2 \), one requires exactly solvable models in order to obtain analytic expressions [2-4]. The scalar curvature has already been calculated for an Ising chain with the result that the curvature \( R \) is positive definite and diverges only at \( T_c = 0 \). In this case, our results following from the Bethe approximation are completely identical with the corresponding exact results.

**Proposition 2.** For an infinite number of neighbours \( (\gamma \to \infty) \), from (17) we simply obtain \( R = \frac{9}{2\delta^2} \) and hence \( R \to \infty \) as \( \delta \to 0 \). This indicates that our theory for scalar curvature goes over exactly into that of mean-field one, reported in Refs. [2, 4], as we increase the value of \( \gamma \).

Above results allow us to interpret the inverse of the curvature expression \( (1/R) \) as a measure of the stability of the spin system. As it is well known, the criteria of stability are expressed through the second derivatives of thermodynamic potentials [2]. Here \( R \) is a function of the second (or higher) order derivatives of the free energy and hence \( 1/R \) is a measure of stability of higher order. For a magnetic system, another interpretation of \( R \) is the quantity proportional to the correlation length.

5. Conclusion

We have evaluated thermodynamic scalar curvature for the Ising model which is a system of spin-1/2 particles. We first considered the free energy expression based on the Bethe’s theory of order-disorder transformation where two order parameters exist and introduced a metric onto the space of these parameters. This is a novel form of metric definition related to the magnetic systems. An expression for Riemannian scalar curvature is then derived according to the scheme described in Section 3. It is found that the curvature obtained has a singularity and diverges to infinity at the critical temperature. This result is consistent with the previously developed analysis of the metric and geometrical structure for the Ising chain and mean-field Ising model. We hope that above perspective on \( R \) may be extended to other various spin systems known in equilibrium statistical mechanics (with more than one order parameter) and used as verifying test for the critical and multicritical phenomena in these models.

Acknowledgments

The author acknowledges support from the Scientific Research Projects Coordination Unit of Akdeniz University. He also thanks Dr. U. Camcı for his kind help during the derivations of the equations at the early stages of this work.
References

[1] Ising E 1925 Beitrag zur Theorie des Ferromagnetismus Zeitschrift für Physik 31 253-258.
[2] Janyszek H and Mrugala R 1989 Riemannian geometry and the thermodynamics of model magnetic systems Phys. Rev. A 39(12) 6515-6523.
[3] Ruppeiner G 1995 Riemannian geometry in thermodynamic fluctuation theory Rev. Mod. Phys. 67 605-659.
[4] Brody D and Rivier N 1995 Geometrical aspects of statistical mechanics Phys. Rev. E 51(2) 1006-1011.
[5] Brody D C and Ritz A 2003 Information geometry of finite Ising models J. Geom. Phys. 47 207-220.
[6] Janke W, Johnston D A and Kenna R 2004 Information geometry and phase transitions Physica A 336 181-1864.
[7] Dey A, Roy P and Sarkar T 2013 Information geometry, phase transitions, and the Widom line: Magnetic and liquids systems Physica A 392 6341-6352.
[8] Ruppeiner G and Bellucci S 2015 Thermodynamic curvature for a two-parameter spin model with frustration Phys. Rev. E 91 012116.
[9] Muto T and Takagi Y 1955 The theory of order-disorder transitions in alloys Solid State Phys. 1 193-282.
[10] Tanaka T, Meijer P H E, and Barry J H 1962 Theory of relaxation phenomena near the second-order phase-transition point J. Chem. Phys. 37(7) 1397-1402.
[11] Barry J H 1966 Magnetic relaxation near a second-order phase transition point J. Chem. Phys. 45(11) 4172-4177.
[12] Ruppeiner G and Davis C 1990 Thermodynamic curvature of the multicomponent ideal gas Phys. Rev. A 41(4) 2200-2202.
[13] Barry J H and Harrington D A 1971 Theory of relaxation phenomena in Ising antiferromagnets Phys. Rev. B 4(9) 3068-3077.