Kosterlitz-Thouless Universality in a Fermionic System

Shailesh Chandrasekharan and James C. Osborn

Department of Physics, Box 90305, Duke University, Durham, North Carolina 27708, USA

(Dated: September 21, 2001)

A new extension of the attractive Hubbard model is constructed to study the critical behavior near a finite temperature superconducting phase transition in two dimensions using the recently developed meron-cluster algorithm. Unlike previous calculations in the attractive Hubbard model which were limited to small lattices, the new algorithm is used to study the critical behavior on lattices as large as $128 \times 128$. These precise results for the first time show that a fermionic system can undergo a finite temperature phase transition whose critical behavior is well described by the predictions of Kosterlitz and Thouless almost three decades ago. In particular it is confirmed that the spatial winding number susceptibility obeys the well known predictions of finite size scaling for $T < T_c$ and up to logarithmic corrections the pair susceptibility scales as $L^{2-\eta}$ at large volumes with $0 \leq \eta \leq 0.25$ for $0 \leq T \leq T_c$.

PACS numbers: 05.30.Fk, 71.10.-w, 67.40.-w, 74.20.-z
Keywords: Superconductivity, Kosterlitz-Thouless Transition, Algorithms, Hubbard Model

INTRODUCTION

A variety of critical phenomena in nature arise due to the development of long range correlations or long range order at a finite temperature. In the critical region quantities are characterized by scaling relations that are universal and depend only on the symmetries involved. The basis for this universality is the renormalization group analysis [1]. A number of universal properties have been confirmed with great precision by numerically studying similar symmetry breaking patterns in different microscopic models. However, almost all known examples involve bosonic variables in the form of either classical [2] or quantum spins [3] at the microscopic level. On the other hand, most interesting physical systems in condensed matter and high energy physics fundamentally involve fermionic particles interacting with each other through gauge fields. Unfortunately, calculations confirming the predictions of universality in such systems are rather limited and crude. In particular precise calculations substantiating the universal critical behavior in superconducting materials or strongly interacting matter cannot be found. The essential difficulty is that the only known approach to study this subject is through numerical simulations. In the case of Fermi systems one has to be clever and overcome the so called sign problem which makes designing algorithms difficult. Even in cases where the sign problem can be solved by integrating out fermions, the conventional algorithms often suffer from critical slowing down. These difficulties have restricted the calculations to small system sizes which are not sufficient to accurately determine the scaling behavior near a phase transition.

The lack of efficient numerical methods available for Fermi systems has created some interesting controversies. It is well known that long range fermionic correlations can arise at zero temperature and can lead to novel universality classes [4]. On the other hand it is believed that the long range degrees of freedom near a finite temperature phase transition should be well described by bosonic degrees of freedom, the reason being that fermions acquire a mass proportional to the temperature $T$ and hence decouple from the critical behavior. However, a few years ago this conventional wisdom was questioned based on a large $N$ calculation and further substantiated by numerical simulations [9] at smaller $N$. It was suggested that the composite nature of the order parameter in fermionic systems may cause deviations from conventional universality. More recently a detailed study of the transition revealed that the deviations could be related to the artifacts of the large $N$ limit [10]. Thus, although the controversy for the moment appears settled the lesson one learns is that universality classes arising in fermionic theories can only be confirmed through precise non-perturbative calculations.

Recently a new method called the meron-cluster algorithm has emerged as a very efficient alternative to solve certain classes of fermionic models [11, 12]. It is based on the well known loop cluster algorithm for quantum spin models [13] and does not suffer from critical slowing down. Using the concept of a meron-cluster it solves the sign problem [14]. This novel method has lead to the first successful determination of the critical behavior near a three dimensional Ising transition in a fermionic model, again confirming the predictions of universality [13, 14]. The calculations of [11] mentioned earlier, had reproduced the two dimensional Ising universality class from large (even) $N$ fermionic systems. This has now been extended to $N = 1$ fermions using a meron-cluster method [15]. As far as we know, until now no one has been able to check the universality arguments with precision beyond the Ising universality class starting from a microscopic fermionic model. In this letter we present the first results from a meron-cluster algorithm which
confirms that the critical behavior near a finite temperature phase transition in a model consisting of fermions can be described by the Kosterlitz-Thouless (KT) universality class [4].

The importance of the KT universality class is well known. A variety of finite temperature phase transitions that arise in many two dimensional condensed matter systems involving phenomena like magnetism, superconductivity and superfluidity are expected to be described by this class. For example the superfluid transition in He\(^4\) occurs due to a condensation of Helium atoms which in reality are tightly bound objects of fermionic constituents. Similarly the superconducting transition in high \(T_c\) materials is expected to occur due to a condensation of electron pairs. Both these transitions are expected to follow the predictions of Kosterlitz and Thouless and are related to a \(U(1)\) particle number symmetry. Although KT universality has been studied extensively using spin systems, it has been difficult to perform precise calculations confirming that a KT universality can arise starting from a microscopic fermionic Hamiltonian. A simple model that has been studied in this context by conventional Monte Carlo methods is the attractive Hubbard model [15, 16]. Unfortunately the inefficiencies of conventional Monte Carlo methods is the attractive Hubbard Hamilton operator in two dimensions and is given by

\[
H = \sum_{<xy>} \sum_{s=\uparrow,\downarrow} (c_{x,s}^\dagger c_{y,s} + c_{y,s}^\dagger c_{x,s})(1 - 3n_{xy} + n_{xy}^2)
- 4 \left(n_{x,\uparrow} - \frac{1}{2}\right) \left(n_{x,\downarrow} - \frac{1}{2}\right) \left(n_{y,\uparrow} - \frac{1}{2}\right) \left(n_{y,\downarrow} - \frac{1}{2}\right)
+ 4 \left[\vec{S}_x \cdot \vec{S}_y + \vec{J}_x \cdot \vec{J}_y - J_3^3 r_{3y}\right]
- 4 \sum_x \left(n_{x,\uparrow} - \frac{1}{2}\right) \left(n_{x,\downarrow} - \frac{1}{2}\right). \tag{1}
\]

Here \(<xy>\) represents the nearest neighbor sites of a square lattice of size \(L \times L\) and \(n_{xy} = n_{x,\uparrow} + n_{x,\downarrow} + n_{y,\uparrow} + n_{y,\downarrow}\). Although the Hamilton operator has many terms, it is easy to check that it is invariant under \(SU(2)\) spin transformations and conserves \(U(1)\) fermion number. Further, there is an on-site attraction between electrons of opposite spins like in the attractive Hubbard model. As we will see, below a critical temperature transportation of fermion number through the bulk becomes easy, leading to superconductivity (or more appropriately superfluidity since the symmetry is not gauged in the model). In higher dimensions this is related to the spontaneous breaking of the \(U(1)\) fermion number symmetry. In two dimensions, since this is forbidden due to the Mermin-Wagner theorem, superconductivity occurs due to the KT phenomena.

The essential feature of the model that makes it useful is the fact that its partition function can be written in terms of the statistical mechanics of closed loops with positive weights [18]. To see this we start with a discrete imaginary time approximation of the partition function

\[
Z = \text{Tr} [\exp(-H/T)] \cong \text{Tr} \left[ \prod_{i=1}^{4} (1 - \varepsilon H_i)^{M} \right] \tag{2}
\]

where \(\varepsilon = 1/(TM)\) and \(H = H_1 + H_2 + H_3 + H_4\) is a convenient reorganization of the interactions present in the Hamiltonian. It is then possible to rewrite the path integral in terms of closed loops with

\[
Z = \sum_{[b]} W[b] \text{Sign}[b] \tag{3}
\]

where \([b]\) is a configuration of bonds linking neighboring sites which form closed loop clusters of sites. The magnitude of the Boltzmann weight is \(W[b] > 0\). The fermion permutation sign is encoded in the topology of the loops. When a configuration contains loops of certain topology, referred to as merons, then \(\text{Sign}[b] = 0\). If there are no meron loops in a configuration then \(\text{Sign}[b] = 2^{N_C}\) where \(N_C\) is the number of loop clusters in the configuration. This novel representation of the partition function makes the model computationally tractable. More details on the meron-cluster formulation can be found in [18].

The approximate partition function given in eq. (3) becomes exact in the limit \(M \to \infty\). Although this continuous time limit can be taken [19], for simplicity the results presented here are obtained by fixing \(M = 20\). In the study of finite temperature critical behavior a sufficiently large but finite \(M\) is acceptable. This is due to the fact that critical dynamics arise from large spatial sizes and the discrete nature of the temporal direction only affects non-universal quantities. The two dimensional universal critical behavior near \(T_c\) remains unaffected.
RESULTS

The simplest observable relevant to superconductivity is the pair susceptibility which we define as

$$\chi = \frac{2T}{ZV} \int_0^{1/T} dt \, \text{Tr} \left[ e^{-(1/T-t)H} p^+ e^{-tH} p^- \right]$$  \quad (4)$$

with $p^+ = \sum_{x} c_{x,\uparrow}^{\dagger} c_{x,\downarrow}$ the pair creation and $p^- = (p^+)^\dagger$ the pair annihilation operators. The susceptibility contains information about the condensation of electron pairs which are the on-site component of Cooper pairs in the BCS approach. A formula for the susceptibility in terms of loop clusters is easy to construct using the results of [20]. In the present case, as discussed in [18], the susceptibility is proportional to the sum over the square of the size of certain clusters depending on the number of meron clusters in the configuration. In figure 1 we show results for the pair susceptibility as a function of spatial size $L$. A state with quasi-long range correlations can be seen as a divergence in the susceptibility. Typically, for temperatures above the superconducting transition temperature $T_c$, the pair susceptibility should reach a constant for large enough volumes. This can be seen for $T = 1.538$ and $T = 1.429$, although in the latter case lattices of size $L = 128$ are necessary to see the saturation suggesting that the correlation lengths may be on the order of 100 lattice units. This dramatic change in the correlation length between $T = 1.538$ and $T = 1.429$ is consistent with a Kosterlitz-Thouless prediction that it should diverge as $\exp(\text{Constant}/\sqrt{T - T_c})$ close to the critical temperature [14]. Interestingly, a fit to a power law over the range $L < 128$ is also poor at $T = 1.429$.

Below $T_c$ the susceptibility should diverge as

$$\chi \propto L^{2-\eta(T)}$$  \quad (5)$$

with the critical exponent $\eta$ starting at $1/4$ at $T_c$ and going down to 0 as $T$ approaches zero. The exact formula has a logarithmic correction to the power law which is small and cannot be accurately determined with reasonable-size lattices so we ignore it here. This continuous change in the power is also clearly visible. We find that $(2 - \eta)$ is $1.767(2)$ at $T = 1.295$ and $1.918(3)$ at $T = 0.5$.

The fits to a power law are extremely good for both these temperatures over the entire range of $L$.

![Figure 1: Pair susceptibility as a function of L.](image1)

**FIG. 1:** Pair susceptibility as a function of $L$.

Although the pair susceptibility alone is sufficient to test for the Kosterlitz-Thouless predictions, there could always be a lingering doubt whether the power law fits would fail when one goes to much larger lattices. For example if we only had data for $L \leq 32$, a power law fit could even work well for $T = 1.429$ when the error bars are sufficiently large. Larger lattices were crucial to determine that the power law was not a good fit in that case. In order to alleviate such worries we looked at the winding number susceptibility which we define as

$$\langle W^2 \rangle = \langle (W_x/2)^2 + (W_y/2)^2 \rangle / 2$$  \quad (6)$$

where $W_x$ ($W_y$) is the total number of fermions winding around the boundary in the $x$ ($y$) direction. This quantity is very useful in measuring $T_c$ and has been used in bosonic systems [21]. Although it is a difficult quantity to measure with conventional algorithms, it is relatively easy in the meron-cluster approach showing the power of the new method. Further, we know its finite size scaling form to be

$$\pi \langle W^2 \rangle = 2 + \sqrt{\Delta(T)} \coth(\sqrt{\Delta(T)} \log(L/L_0(T)))$$  \quad (7)$$

with $\Delta(T_c) = 0$ [22]. It can be shown that for $T < T_c$ in the $L \to \infty$ limit $2\pi \eta(T) \langle W^2 \rangle = 1$ [21, 23]. The

![Figure 2: Comparison between $\eta(T)$ and $1/2\pi \langle W^2 \rangle$ as a function of $T$.](image2)

**FIG. 2:** Comparison between $\eta(T)$ and $1/2\pi \langle W^2 \rangle$ as a function of $T$. 

Below $T_c$ the susceptibility should diverge as $L^{2-\eta(T)}$ with the critical exponent $\eta$ starting at $1/4$ at $T_c$ and going down to 0 as $T$ approaches zero.
fact that \( (W^2) \) jumps to the universal number \( 2/\pi \) from 0 is another well known feature of the KT phenomena and can be used to determine \( T_c \). Since \( \eta(T) \) can be determined from the scaling of the pair susceptibility one can combine it with the measurement of \( (W^2) \) below \( T_c \) to check for consistency in the KT universality class. Figure 2 compares \( 1/(2\pi(W^2)) \) obtained by extrapolating the values of the winding number susceptibility to the infinite volume limit using the formula (3) and \( \eta(T) \) obtained from the finite size scaling of the pairing susceptibility, as a function of temperature. Clearly the results are in excellent agreement with the predictions for a KT phase transition.

**DIRECTIONS FOR THE FUTURE**

This work can be extended in several directions. One interesting problem in condensed matter physics is to understand how disorder effects superconductivity. It is predicted that at zero temperature as the disorder is increased the system undergoes a quantum phase transition to an insulating phase [24]. If this is indeed the case, it would be interesting to understand the underlying critical behavior starting from a fermionic theory. Previous studies have used the attractive Hubbard model as the starting point [25]. We suggest that the model studied here is perhaps a better alternative since the meron-cluster algorithms could turn out to be more efficient in such a study. Many other fermionic models with continuous symmetries and applications in condensed matter, nuclear and high energy physics can be studied with meron-cluster techniques. Whether there is d-wave superconductivity in these models is an open question. A common feature of these new models is that they appear to be more complicated. However since we have algorithms for them which give a computational advantage, they may still produce the clearest results. It is a common practice to work with models that are the easiest to solve (numerically in this case) to help understand complicated physical systems. Once the basic phenomena is understood one can then attempt more difficult models to explore the robustness and variations in the details of the underlying physics.

**Acknowledgments**

We thank Uwe-Jens Wiese and Harold Baranger for many fruitful discussions. We also thank Xincheng Xie and Richard Scalettar for clarifications about the physics of the Hubbard model. This work is supported in part by funds provided by the U.S. Department of Energy grant DE-FG02-96ER40945 and the National Science Foundation grant DMR-0103003. The computations were performed on **Brahma**, a Pentium based Beowulf cluster constructed using computers donated generously by the Intel Corporation and located in the physics department at Duke University.

---

[1] E. H. Stanley, Rev. Mod. Phys. 71, 358 (1999).
[2] M. Campostrini, et.al., Phys. Rev. B 63 214503 (2001); Nucl. Phys. Proc. Suppl. 94 857-860 2001.
[3] B. Beard, et.al., Phys. Rev. Lett. 80, 1742 (1998).
[4] B. Rosenstein, B.J. Warr and S.H. Park, Phys. Rep. 205 59 (1991).
[5] A. Kocic and J. Kogut, Phys. Rev. Lett. 74, 3109 (1995); Nucl. Phys. B455, 229 (1995).
[6] J.B. Kogut, M.A. Stephanov and C.G. Strouhos, Phys. Rev. D 58 096001 (1998).
[7] S. Chandrasekharan and U.-J. Wiese, Phys. Rev. Lett. 83, 3116 (1999).
[8] S. Chandrasekharan, Nucl. Phys. (Proc. Suppl.) 83-84, 774 (2000).
[9] H. G. Evertz, G. Lana and M. Marcu, Phys. Rev. Lett. 70 875 (1993).
[10] W. Bietenholz, A. Pochinsky and U.-J. Wiese, Phys. Rev. Lett. 75 4524 (1995).
[11] S. Chandrasekharan, J. Cox, K. Holland and U.-J. Wiese, Nucl. Phys. B576, 481 (2000).
[12] S. Chandrasekharan and J. C. Osborn, Phys. Lett. B496, 122 (2000).
[13] J. Cox and K. Holland, Nucl. Phys. B583, 331 (2000).
[14] J. M. Kosterlitz and D. J. Thouless, J. Phys. C 6, 1181 (1973).
[15] R. Scalettar et al., Phys. Rev. Lett. 62 1407 (1989).
[16] A. Moreo and D. J. Scalapino, Phys. Rev. Lett. 66 946 (1991).
[17] R. Lacaze, A. Morel, B. Petersson and J. Schröper, Eur. Phys. J. B2, 509 (1998).
[18] S. Chandrasekharan, J. Cox, J.C. Osborn and U.-J. Wiese, in preparation
[19] B. B. Beard and U.-J. Wiese, Phys. Rev. Lett. 77 5130 (1996).
[20] R. Brower, S. Chandrasekharan and U.-J. Wiese, Physica A261 520 (1998).
[21] E.L. Pollock and D.M. Ceperley, Phys. Rev. B 36 8343 (1987);
[22] K. Harada and N. Kawashima, J. Phys. Soc. Jpn. 67 (1998) 2768.
[23] D.R. Nelson and J. M. Kosterlitz, Phys. Rev. Lett. 39 1201 (1977).
[24] A. M. Goldman and N. Marković, Physics Today, 30, November 1998.
[25] R. Scalettar, N. Trivedi and C. Huscroft, Phys. Rev B59, 4364 (1999).