Cluster Percolation and Chiral Phase Transition

Matteo Becucci\textsuperscript{a,b}, Antonio Moro\textsuperscript{a,b}

\textsuperscript{a} Dipartimento di Fisica dell’Università di Lecce, I-73100, Italy,
\textsuperscript{b} Istituto Nazionale di Fisica Nucleare - INFN, Sezione di Lecce

The Meron Cluster algorithm solves the sign problem in a class of interacting fermion lattice models with a chiral phase transition. Within this framework, we study the geometrical features of the clusters built by the algorithm, that suggest the occurrence of a generalized percolating phase transition at the chiral critical temperature in close analogy with Fortuin-Kasteleyn percolation in spin models.

PACS numbers: 71.10.Fd, 64.60.Ak

A fundamental difficulty in the Monte Carlo study of fermion lattice models is the sign problem due to the fluctuating sign of the statistical weight of fermion configurations. Recently, the Meron Cluster algorithm (MCA)\footnote{MCA} has been proposed as an effective solution to the sign problem in a class of interacting models. In particular, here, we focus on a 2 + 1 dimensional model with a second order phase transition associated to the dynamical breaking of a discrete chiral symmetry\footnote{Discrete chiral symmetry breaking in lattice fermion models}\footnote{Cluster dynamics and look for critical phenomena defined in terms of cluster shapes.}. The simplest example of such a scenario is the 2D Ising model with a second order phase transition at the critical temperature in close analogy with Fortuin-Kasteleyn percolation\footnote{Fortuin-Kasteleyn percolation in the clusters built by the algorithm, that suggest the occurrence of a generalized percolating phase transition}. The Meron Cluster algorithm solves the sign problem in a class of interacting fermion lattice models, hopping on a 2 + 1 dimensional lattice with $L^2$ spatial sites, described in\footnote{Fermions, hopping on a 2 + 1 dimensional lattice with $L^2$ spatial sites}. The Hamiltonian is

\begin{equation}
H = \sum_x \sum_{i=1,2} \{\eta_{x,i}(c_{x}^\dagger c_{x+i} + h.c.) + \}
\end{equation}

\begin{equation}
+ G \left( n_x - \frac{1}{2} \right) \left( n_{x+i} - \frac{1}{2} \right)
\end{equation}

where $n_x = c_x^\dagger c_x$ is the occupation number at site $x$, $\eta_{x,i}$ are the Kawamoto-Smit phases $\eta_{x,1} = 1$, $\eta_{x,2} = (-1)^{\hat{\sigma}_x}$ and the operators $c^\dagger$ obey standard anti-commutation relations $\{c_x, c_y\} = 0$, $\{c_x^\dagger, c_y^\dagger\} = \delta_{x,y}$. In the following we shall consider the case $G = 1$ and adopt periodic boundary conditions.

The partition function $\text{Tr} e^{-\beta H}$ can be computed by Trotter splitting that maps the quantum model to a statistical system on a 2 + 1 dimensional lattice with $L^2 \times T$ sites. The temporal lattice spacing is $\varepsilon = 4\beta/T$. The limit $\varepsilon \to 0$ must be taken at fixed $\beta$ with $T \to \infty$. In practice, we shall present results obtained at the fixed value $T = 40$ where $\beta$ can cover the transition point with reasonably small $\varepsilon$. Each configuration is specified by the occupation numbers $n_x = \{n_{x,t}\}$ and carries a sign $\sigma(n) = \pm 1$, source of the sign-problem. To update a configuration, sites are clustered according to definite rules depending on $\beta$ and discussed in details in\footnote{Clustered algorithm clusters and underlying physical thermal transition}. Each cluster is then independently flipped: with probability 1/2 we apply the global transformation $n_{x,t} \to 1 - n_{x,t}$ to all of its sites. Clusters
whose flip changes $\sigma(n)$ are defined merons.

The chiral phase transition can be analyzed by studying the asymptotic volume dependence of the susceptibility $\chi$. Defining the chiral condensate in the configuration $n = (n_x, t)$ as

$$Z(n) = \xi \sum_{x,t} (-1)^{x_1+x_2} \left( n_{x,t} - \frac{1}{2} \right),$$

the chiral susceptibility $\chi$ is given by

$$\chi = \frac{1}{\beta L^2} \frac{\langle (Z(n))^2 \rangle}{\langle \sigma(n) \rangle}.$$  \hfill (4)

An improved estimator of $\chi$ free of sign problems can be built by writing $Z(n)$ as a sum over clusters $Z(n) = \sum_C Z_C$ and taking its average over $2^{N_C}$ possible flips, where $N_C$ is the number of the clusters. Then, $\chi$ gets contributions from sectors with meron number $N = 0, 2$:

$$\chi = \frac{1}{\beta L^2} \frac{\langle \sum_C Z_C^2 \delta_{N,0} + 2 |Z_C Z_{C'}| \delta_{N,2} \rangle}{\langle \delta_{N,0} \rangle},$$

where, for $N = 2$, $C_1$, $C_2$ are the two merons.

From numerical simulations, apart from rather small scaling violations, $\chi$ obeys the Finite Size Scaling (FSS) law $\chi = L^\gamma f_{\chi}(L(\beta - \beta_{th}))$ with the exponent $\gamma = 7/4$, characteristic of the 2D Ising universality class \textsuperscript{[2]}.

Numerical simulations locate the chiral $\beta$ at $\beta_{th} = 2.43(1)\textsuperscript{[3]}$ (the subscript “th” stands for “thermal”).

To detect a possible purely geometrical transition, we study quantities $Q$ that depend only on the cluster shape and not on their internal occupation numbers. Since cluster flips do not change $Q$ and meron flips change the sign of $\sigma(n)$, the improved estimator of $Q$ is

$$\frac{\langle Q(n) \sigma(n) \rangle}{\langle \sigma(n) \rangle} = \frac{\langle Q(n) \delta_{N,0} \rangle}{\langle \delta_{N,0} \rangle} = E_0(Q),$$

that is the average restricted to the zero meron sector.

The simplest set of geometrical quantities that we can study are the moments $M_n = E_0(\sum_C |C|^n)$ of the normalized cluster size $|C| = Vol(C)/T$ where Vol($C$) is the number of sites in $C$.

![Fig. 1. FSS analysis of $M_n$ and $E_0(max|C|)$.](image1)

We perform simulations to compute numerically $\{M_n\}_{n=2,3,4}$ and also $E_0(max|C|)$. We work on lattices with $L = 8, 10, 12, 14, 16$ in the range $1.5 < \beta < 3.0$ and presented about $1.5 \cdot 10^5$ measures per point. Fig. \textsuperscript{[4]} shows the numerical data supporting as a first result the remarkable validity of the empirical scaling relations:

$$\beta^{n/2} M_n = L^{n\rho} f_n(y), \quad n \geq 2,$$

$$\beta^{1/2} E_0(\max|C|) = L^\rho h(y)$$

in terms of the scaling variable $y = L(\beta - \beta_c)$.

To detect a possible purely geometrical transition, we find $\beta_c \approx \beta_{th}$ with an accuracy that can be appreciated by looking at Fig. \textsuperscript{[2]}.

![Fig. 2. Data crossing for $M_2$ with different $L$. By virtue of the scaling law Eq. (7), at $\beta = \beta_c$ the quantity $\beta M_2 L^{-2\rho}$ is independent on $L$.](image2)

The ratios $R_n = M_2^{1/2}/M_n^{1/n}$ for $n = 3, 4$ and $R_\infty = M_2^{1/2}/E_0(\max|C|)$ are shown in Fig. \textsuperscript{[5]}.
FIG. 3. Ratios $R_n$ and $R_\infty$. $M_n^{1/n}$ is well approximated by the contribution of the largest cluster beyond the critical point.

The plots strongly indicate that $R_n$ are independent on $L$ at fixed $y$ in agreement with Eq. (7).

It can be checked that, at $\beta = \beta_c$, $M_n$ receives the main contribution from a small set of large clusters growing like $L^{\rho}$, and the fact that the ratios $R_n(y) \rightarrow 1$ as $y$ grows, simply means that this contribution is more and more dominant. We briefly summarize this behavior by saying that the clusters are percolating. Following [13], further information on the critical ensemble can be obtained by studying the cluster distribution

$$n_s = \mathbb{E}_0(\text{\# number of clusters } C \text{ with } \text{Vol}(C) = s).$$

In Fig. (4) we show that the simple law

$$n_s = L^{-\rho} f \left( \frac{s}{L^\rho} \right),$$

is well satisfied for $s/L^\rho \gg 1$.

The critical cluster distribution $n_s$ decreases not faster than algebraically with $s$ until $s \approx 40 L^\rho$ where the final large cluster tail is reached and $n_s$ falls down quickly.

If one takes into account that the leading contribution to $\{M_n\}_{n \geq 2}$ actually comes from the region where $s/L^\rho \gg 1$, observing that $M_n = \sum_s s^n n_s$ and using Eq. (9) we obtain a $L$-dependence consistent with Eq. (7).

There are many small clusters and one can check that the normalized number of clusters $\beta \mathbb{E}_0(N_C)/L^2$ depends mildly on $L$ for a wide range of $\beta$ and $L$.

It is interesting to analyze what happens to the typical cluster configurations when $\beta$ is gradually increased toward the critical point. At small $\beta$, almost all bonds that build the clusters are set in the temporal direction. In physical terms the fermions hop from the initial positions to neighboring ones with small probability. Sites simply tend to cluster in $L^2$ straight vertical lines with $T$ sites. As $\beta \rightarrow \beta_c$, the vertical clusters start merging and breaking and form complicated structures with large dispersion in the cluster size distribution. This process can be seen in Fig. (5):

![FIG. 5. Two elementary clusters with equal dimension $T$, first merge into a single cluster, then break apart in two clusters with very different dimension.](image)

Two vertical clusters with Vol($C$) = $T$ undergo a two step process allowed by the cluster rules [2]. In the end, they give rise to a large cluster with Vol($C$) = $2T - 4$ and a small one with 4 sites. After many processes of this kind we find a few large clusters surrounded by a gas of smaller clusters. In Fig. (6) we show a typical largest cluster obtained at $\beta = 2.5$ on the $8^2 \times 40$ lattice.

![FIG. 6. A typical largest link configuration for the $8^2 \times 40$ lattice at $\beta = \beta_c$.](image)

Geometrical quantities that can measure this dispersion effect are the cumulants $\{G_n\}_{n \geq 1}$ of the cluster size.
distribution defined as
\[ \sum_{n \geq 1} \frac{\lambda^n}{n!} G_n = E_0 \left\{ \log \left( \sum_{n \geq 0} \frac{\lambda^n}{n!} \sum_{C} \frac{1}{N_C} \sum_{|C|} |C|^n \right) \right\}. \] (10)

In our study we do not consider the cumulant \( G_1 \), whose behavior is determined by the the contributions from small clusters, with \( s \ll L^\beta \).

The next cumulant is the variance
\[ G_2 = E_0 \left( \frac{1}{N_C} \sum_{C} |C|^2 - \frac{1}{N_C^2} \left( \sum_{C} |C| \right)^2 \right). \] (11)

Our data support a FSS law of the form
\[ \beta G_2 = L^{\rho} g_2(y), \] (12)
with \( \rho' = 1.51(4) \), which is compatible with \( 2\gamma - 2 \). This exponent can be explained taking account that, analogously to the moment \( M_2 \), the contributions from small clusters are negligible and that, within errors, \( \sum_{C} |C|^2 \sim L^{2\gamma} \) and \( N_C \sim L^2 \).

As we remarked above, when \( \beta \to 0 \), the clusters are simple vertical lines and \( G_2 \to 0 \) like \( \chi \) does. This fact suggests that it could be interesting to study a possible relationship between these quantities at different \( \beta \) values. We remark that, in principle, \( G_2 \) and \( \chi \) have different topological origins: \( \chi \) is calculated on zero and two merons sector, while \( G_2 \) only on zero-meron sector. Nevertheless, we find that the following empirical relation
\[ \chi \simeq 0.15(1) \cdot (\beta G_2)^{\frac{3}{2} - \gamma}, \] (13)
holds for a wide range of parameters \((L, \beta)\) as shown in Fig. (7).

![Graph](image-url)

**FIG. 7.** Comparison between \( \chi \) (empty symbols) and \( 0.15 \cdot (\beta G_2)^{3/2} \) (full symbols).

In practice, in the region that we have explored, the ratio \( \chi/(\beta G_2)^{3/2} \) is consistent, within errors, with a constant. This result signals an unexpected correlation between different topological sectors. In particular, Eq. (13) could be relevant in the construction of a purely geometrical definition of \( \chi \). A FSS study of the higher cumulants \( G_3 \) and \( G_4 \) shows similar scaling laws, but with exponents that are not in simple relation with \( \gamma \) and should in principle be matched to the anomalous dimensions of higher operators in the 2D Ising universality class.

To conclude, we have examined the critical behavior of the clusters that arise in the application of the Meron algorithm to a fermion model in \( 2 + 1 \) dimensions. We have found simple FSS laws that we have explained in terms of a percolative process occurring at the chiral critical temperature. Our data support the results \( \rho \simeq \gamma, \rho' \simeq 2\gamma - 2 \), as well as the empirical relation Eq. (13) that shows a close correlation between physical and geometrical quantities.

We acknowledge S. Chandrasekharan, K. Holland and U.J. Wiese for useful discussions about the Meron-Cluster Algorithm and its applications. Financial support from INFN, IS-RM42 is also acknowledged.

[1] W. von der Linden, Phys. Rep. 220, 53 (1992).
[2] S. Chandrasekharan and J. Osborn, Springer Proc. Phys. 86, 28 (2000); S. Chandrasekharan and J. C. Osborn, Phys. Lett. B 496, 122 (2000); S. Chandrasekharan, Chin. J. Phys. 38, 696 (2000); S. Chandrasekharan, Nucl. Phys. Proc. Suppl. 83, 774 (2000); S. Chandrasekharan and U. J. Wiese, Phys. Rev. Lett. 83, 3116 (1999); S. Chandrasekharan, Nucl. Phys. Proc. Suppl. 106, 1025 (2002);
[3] S. Chandrasekharan, J. Cox, K. Holland and U. J. Wiese, Nucl. Phys. B 576, 481 (2000);
[4] J. Cox and K. Holland, Nucl. Phys. B 583, 331 (2000).
[5] P. W. Kasteleyn, C. M. Fortuin, Jour. Phys. Soc. of Japan 26 (Suppl.), 11 (1969); C. M. Fortuin, P. W. Kasteleyn, Physica 57, 536 (1972); C. M. Fortuin, Physica 58, 393 (1972); C. M. Fortuin, Physica 59, 545 (1972).
[6] R. G. Edwards, A. D. Sokal, Phys. Rev. D 38, 2009 (1988).
[7] S. Fortunato, H. Satz, Nucl. Phys. Proc. Suppl. 106, 890 (2002); S. Fortunato, F. Karsch, P. Petreczky and H. Satz, Nucl. Phys. Proc. Suppl. 94, 398 (2001); S. Fortunato and H. Satz, Nucl. Phys. B 598, 601 (2001). P. Blanchard et al., J. Phys. A 33, 8603 (2000);
[8] A. Coniglio, C. R. Nappi, F. Peruggi and L. Russo, Commun. Math. Phys. 51, 315 (1976).
[9] M. F. Sykes, D. S. Gaunt, Jour. of Phys. A 9, 2131 (1976).
[10] H. Müller-Krumbhaar, Phys. Lett. A 48, 459 (1974).
[11] A. Coniglio, W. Klein, Jour. of Phys. A 13, 2775 (1980).
[12] The first numerical evidence of this result is J. B. Kogut, M. A. Stephanov, C.G. Strouthos, Phys. Rev. D 58, 096001 (1998);
[13] D. Stauffer, Phys. Rept. 54, 1 (1979).