2D Ising Model with MCMC: Group B

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In this project, we use a MCMC method to simulate a 2D Ising spin lattice in varying magnetic fields and at varying temperatures. We explore parameters used to set up the simulation and see how certain starting conditions give rise to hysteresis and metastable states at low enough temperatures.

Usage: Secondary publications and information retrieval purposes.

Structure: You may use the description environment to structure your abstract; use the optional argument of the \item command to give the category of each item.

I. INTRODUCTION

Introduction to project

II. ISING MODEL

For this project, we focus on the 2D Ising model, which consists of a lattice of spins $\{+1, -1\}$ and is often used to approximate ferromagnetic materials. The behavior of the system is described by an energy function $E(\sigma)$, where σ represents the configuration of spins. The energy function is defined as:

$$E(\sigma) = -J \sum_{\langle ij \rangle} \sigma_i \sigma_j - B \sum_{i \in 2} \sigma_i \tag{1}$$

Here, J denotes the coupling constant, B represents the external magnetic field, and the terms $\sum_{\langle ij \rangle}$ and $\sum_{i \in 2}$ represent summations over nearest neighbors and all spins, respectively. The symbol $\langle ij \rangle$ signifies pairs of adjacent lattice sites.

The first term $-J\sum_{\langle ij\rangle}\sigma_i\sigma_j$ captures the interaction energy between neighboring spins, where aligned neighbors have lower energy than opposing neighbors. The second term $-B\sum_{i\in 2}\sigma_i$ represents the interaction of spins with the external magnetic field.

A significant consequence of this energy function is the tendency of the lattice to align with the external magnetic field at low temperatures, as spins converge towards the lowest energy state.

Furthermore, the magnetization $M(\sigma)$ of the system, defined as the average spin per site, is given by:

$$M(\sigma) = \frac{1}{|2|} \sum_{i \in 2} \sigma_i \tag{2}$$

Here, |2| represents the total number of lattice sites. Attach some snapshots of low temperature, negative magnetic field; low temperature, positive magnetic field.

III. MONTE CARLO MARKOV CHAIN

Monte Carlo methods describe a broad class of algorithms that attempt to reduce operational complexity and computation time by replacing exhaustive computations with random ones. In this project, instead of computing the full dynamics of the system, which would be intractible, we pick a random cell in the lattice at each time step, and decide whether or not to flip it based on some probability dependent in the projected change in energy, and the predefined "temperature" of the system.

A Markov Chain is a probabilistic state system in which each state has a defined probability to transition to each other state at every time step. These states are often visualized as nodes in a network, with each directed edge weighted according to the probability that the state will move along that edge from its initial to terminal nodes. In computing, this is more often computed as a transition matrix that encodes the same information.

For our purposes, however, we do not necessarily know the full probability matrix, as the phase space for this problem is intractible to solve completely. Instead, we know the transition probability based on the state variables, and need to evolve the system in time based on that. This is where Monte Carlo Markov Chains help. By stepping around the phase space randomly, weighted according to known transition rules, we can more efficiently explore the phase space of the system in an approximate manner.

IV. FIRST-LEVEL HEADING: THE LINE BREAK WAS FORCED via \\

This sample document demonstrates proper use of REVTEX 4.2 (and LATEX 2_{ε}) in manuscripts prepared for submission to APS journals. Further information can be found in the REVTEX 4.2 documentation included in the distribution or available at http://journals.aps.org/revtex/.

When commands are referred to in this example file, they are always shown with their required arguments, using normal TEX format. In this format, #1, #2, etc. stand for required author-supplied arguments to com-

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mands. For example, in \section{#1} the #1 stands for the title text of the author's section heading, and in \title{#1} the #1 stands for the title text of the paper.

Line breaks in section headings at all levels can be introduced using \\. A blank input line tells TEX that the paragraph has ended. Note that top-level section headings are automatically uppercased. If a specific letter or word should appear in lowercase instead, you must escape it using \lowercase{#1} as in the word "via" above.

A. Second-level heading: Formatting

This file may be formatted in either the preprint or reprint style. reprint format mimics final journal output. Either format may be used for submission purposes. letter sized paper should be used when submitting to APS journals.

1. Wide text (A level-3 head)

The widetext environment will make the text the width of the full page, as on page 4. (Note the use the \pageref{#1} command to refer to the page number.)

a. Note (Fourth-level head is run in) The width-changing commands only take effect in two-column formatting. There is no effect if text is in a single column.

B. Citations and References

A citation in text uses the command \cite{#1} or \onlinecite{#1} and refers to an entry in the bibliography. An entry in the bibliography is a reference to another document.

1. Citations

Because REVTEX uses the natbib package of Patrick Daly, the entire repertoire of commands in that package are available for your document; see the natbib documentation for further details. Please note that REVTEX requires version 8.31a or later of natbib.

a. Syntax The argument of \cite may be a single key, or may consist of a comma-separated list of keys. The citation key may contain letters, numbers, the dash (-) character, or the period (.) character. New with natbib 8.3 is an extension to the syntax that allows for a star (*) form and two optional arguments on the citation key itself. The syntax of the \cite command is thus (informally stated)

\cite { key }, or
\cite { optarg+key }, or
\cite { optarg+key , optarg+key...},
where optarg+key signifies

key, or *key, or [pre] key, or [pre] [post] key, or even *[pre] [post] key.

where pre and post is whatever text you wish to place at the beginning and end, respectively, of the bibliographic reference (see Ref. [1] and the two under Ref. [2]). (Keep in mind that no automatic space or punctuation is applied.) It is highly recommended that you put the entire pre or post portion within its own set of braces, for example: $\text{cite } \{ \text{ [} \{text\} \} key \}$. The extra set of braces will keep LaTeX out of trouble if your text contains the comma (,) character.

The star (*) modifier to the *key* signifies that the reference is to be merged with the previous reference into a single bibliographic entry, a common idiom in APS and AIP articles (see below, Ref. [2]). When references are merged in this way, they are separated by a semicolon instead of the period (full stop) that would otherwise appear.

- b. Eliding repeated information When a reference is merged, some of its fields may be elided: for example, when the author matches that of the previous reference, it is omitted. If both author and journal match, both are omitted. If the journal matches, but the author does not, the journal is replaced by *ibid.*, as exemplified by Ref. [2]. These rules embody common editorial practice in APS and AIP journals and will only be in effect if the markup features of the APS and AIP BibTEX styles is employed.
- c. The options of the cite command itself Please note that optional arguments to the key change the reference in the bibliography, not the citation in the body of the document. For the latter, use the optional arguments of the \cite command itself: \cite *[pre-cite] [post-cite] {key-list}.

2. Example citations

By default, citations are numerical[3]. Author-year citations are used when the journal is RMP. To give a textual citation, use \onlinecite{#1}: Refs. 1 and 4. By default, the natbib package automatically sorts your citations into numerical order and "compresses" runs of three or more consecutive numerical citations. REVT_FX provides the ability to automatically change the punctuation when switching between journal styles that provide citations in square brackets and those that use a superscript style instead. This is done through the citeautoscript option. For instance, the journal style prb automatically invokes this option because Physical Review B uses superscript-style citations. The effect is to move the punctuation, which normally comes after a citation in square brackets, to its proper position before the superscript. To illustrate, we cite several together [1, 2, 4-6], and once again in different order

(Refs. [1, 2, 4–6]). Note that the citations were both compressed and sorted. Futhermore, running this sample file under the prb option will move the punctuation to the correct place.

When the prb class option is used, the \cite{#1} command displays the reference's number as a superscript rather than in square brackets. Note that the location of the \cite{#1} command should be adjusted for the reference style: the superscript references in prb style must appear after punctuation; otherwise the reference must appear before any punctuation. This sample was written for the regular (non-prb) citation style. The command \onlinecite{#1} in the prb style also displays the reference on the baseline.

3. References

A reference in the bibliography is specified by a \bibitem{#1} command with the same argument as the \cite{#1} command. \bibitem{#1} commands may be crafted by hand or, preferably, generated by BibTEX. REVTEX 4.2 includes BibTEX style files apsrev4-2.bst, apsrmp4-2.bst appropriate for *Physical Review* and *Reviews of Modern Physics*, respectively.

4. Example references

This sample file employs the \bibliography command, which formats the apssamp.bbl file and specifies which bibliographic databases are to be used by BibTeX (one of these should be by arXiv convention apssamp.bib). Running BibTeX (via bibtex apssamp) after the first pass of LATeX produces the file apssamp.bbl which contains the automatically formatted \biblitem commands (including extra markup information via \biblinfo and \bibfield commands). If not using BibTeX, you will have to create the thebibiliography environment and its \biblitem commands by hand.

Numerous examples of the use of the APS bibliographic entry types appear in the bibliography of this sample document. You can refer to the apssamp.bib file, and compare its information to the formatted bibliography itself.

C. Footnotes

Footnotes, produced using the \footnote{#1} command, usually integrated into the bibliography alongside the other entries. Numerical citation styles do this[7]; author-year citation styles place the footnote at the bottom of the text column. Note: due to the method used to place footnotes in the bibliography, you must re-run BibTEX every time you change any of your document's footnotes.

V. MATH AND EQUATIONS

Inline math may be typeset using the \$\$ delimiters. Bold math symbols may be achieved using the bm package and the \bm{#1} command it supplies. For instance, a bold α can be typeset as $\boldsymbol{\alpha}$ giving $\boldsymbol{\alpha}$. Fraktur and Blackboard (or open face or double struck) characters should be typeset using the \mathfrak{#1} and \mathbb{#1} commands respectively. Both are supplied by the amssymb package. For example, $\boldsymbol{\alpha}$ gives $\boldsymbol{\alpha}$ and $\boldsymbol{\alpha}$ mathbb{R}\$ gives $\boldsymbol{\alpha}$ and $\boldsymbol{\alpha}$ mathfrak{G}\$ gives $\boldsymbol{\alpha}$

In IATEX there are many different ways to display equations, and a few preferred ways are noted below. Displayed math will center by default. Use the class option fleqn to flush equations left.

Below we have numbered single-line equations; this is the most common type of equation in *Physical Review*:

$$\chi_{+}(p) \lesssim \left[2|\mathbf{p}|(|\mathbf{p}|+p_z)\right]^{-1/2} \begin{pmatrix} |\mathbf{p}|+p_z\\ px+ip_y \end{pmatrix}, \quad (3)$$
$$\left\{1234567890abc123\alpha\beta\gamma\delta1234556\alpha\beta\frac{1\sum_{b}^{a}}{A^2}\right\}. \quad (4)$$

Note the open one in Eq. (4).

Not all numbered equations will fit within a narrow column this way. The equation number will move down automatically if it cannot fit on the same line with a one-line equation:

$$\left\{ab12345678abc123456abcdef\alpha\beta\gamma\delta1234556\alpha\beta\frac{1\sum_{b}^{a}}{A^{2}}\right\}.$$
 (5)

When the \label{#1} command is used [cf. input for Eq. (4)], the equation can be referred to in text without knowing the equation number that TEX will assign to it. Just use \ref{#1}, where #1 is the same name that used in the \label{#1} command.

Unnumbered single-line equations can be typeset using the $\[\]$ format:

$$g^+g^+ \to g^+g^+g^+g^+\dots$$
, $q^+q^+ \to q^+g^+g^+\dots$.

A. Multiline equations

Multiline equations are obtained by using the equarray environment. Use the \nonumber command at the end of each line to avoid assigning a number:

$$\mathcal{M} = ig_Z^2 (4E_1 E_2)^{1/2} (l_i^2)^{-1} \delta_{\sigma_1, -\sigma_2} (g_{\sigma_2}^e)^2 \chi_{-\sigma_2}(p_2) \times [\epsilon_j l_i \epsilon_i]_{\sigma_1} \chi_{\sigma_1}(p_1), \tag{6}$$

$$\sum |M_g^{\text{viol}}|^2 = g_S^{2n-4}(Q^2) N^{n-2}(N^2 - 1)$$

$$\times \left(\sum_{i < j}\right) \sum_{\text{perm}} \frac{1}{S_{12}} \frac{1}{S_{12}} \sum_{\tau} c_{\tau}^f . \quad (7)$$

Note: Do not use \label{#1} on a line of a multiline equation if \nonumber is also used on that line. Incorrect cross-referencing will result. Notice the use \text{#1} for using a Roman font within a math environment.

To set a multiline equation without *any* equation numbers, use the \begin{eqnarray*}, \end{eqnarray*} format:

$$\sum |M_g^{\text{viol}}|^2 = g_S^{2n-4}(Q^2) \ N^{n-2}(N^2 - 1)$$

$$\times \left(\sum_{i < j}\right) \left(\sum_{\text{perm}} \frac{1}{S_{12}S_{23}S_{n1}}\right) \frac{1}{S_{12}} \ .$$

To obtain numbers not normally produced by the automatic numbering, use the $\text{tag}\{\text{#1}\}$ command, where #1 is the desired equation number. For example, to get an equation number of (2.6'),

$$q^+q^+ \to q^+q^+q^+q^+ \dots$$
, $q^+q^+ \to q^+q^+q^+ \dots$ (2.6')

a. A few notes on tags \tag{#1} requires the amsmath package. Place the \tag{#1} command before the \label{#1}, if any. The numbering produced by \tag{#1} does not affect the automatic numbering in REVTEX; therefore, the number must be known ahead of time, and it must be manually adjusted if other equations are added. \tag{#1} works with both single-line and multiline equations. \tag{#1} should only be used in exceptional cases—do not use it to number many equations in your paper. Please note that this feature of the

amsmath package is *not* compatible with the hyperref (6.77u) package.

Enclosing display math within \begin{subequations} and \end{subequations} will produce a set of equations that are labeled with letters, as shown in Eqs. (8b) and (8a) below. You may include any number of single-line and multiline equations, although it is probably not a good idea to follow one display math directly after another.

$$\mathcal{M} = ig_Z^2 (4E_1 E_2)^{1/2} (l_i^2)^{-1} (g_{\sigma_2}^e)^2 \chi_{-\sigma_2}(p_2)$$

$$\times [\epsilon_i]_{\sigma_1} \chi_{\sigma_1}(p_1).$$
(8a)

$$\left\{abc123456abcdef\alpha\beta\gamma\delta1234556\alpha\beta\frac{1\sum_{b}^{a}}{A^{2}}\right\},\qquad(8b)$$

Giving a \label{#1} command directly after the \begin{subequations}, allows you to reference all the equations in the subequations environment. For example, the equations in the preceding subequations environment were Eqs. (8).

1. Wide equations

The equation that follows is set in a wide format, i.e., it spans the full page. The wide format is reserved for long equations that cannot easily be set in a single column:

$$\mathcal{R}^{(d)} = g_{\sigma_2}^e \left(\frac{[\Gamma^Z(3,21)]_{\sigma_1}}{Q_{12}^2 - M_W^2} + \frac{[\Gamma^Z(13,2)]_{\sigma_1}}{Q_{13}^2 - M_W^2} \right) + x_W Q_e \left(\frac{[\Gamma^{\gamma}(3,21)]_{\sigma_1}}{Q_{12}^2 - M_W^2} + \frac{[\Gamma^{\gamma}(13,2)]_{\sigma_1}}{Q_{13}^2 - M_W^2} \right). \tag{9}$$

This is typed to show how the output appears in wide format. (Incidentally, since there is no blank line between the equation environment above and the start of this paragraph, this paragraph is not indented.)

VI. CROSS-REFERENCING

REVT_EX will automatically number such things as sections, footnotes, equations, figure captions, and table captions. In order to reference them in text, use the $\label{#1}$ and $\ref{#1}$ commands. To reference a particular page, use the $\pageref{#1}$ command.

The \label{#1} should appear within the section heading, within the footnote text, within the equation, or within the table or figure caption. The \ref{#1} command is used in text at the point where the reference is to be displayed. Some examples: Section IV on page 1, Table I, and Fig. 1.

VII. FLOATS: FIGURES, TABLES, VIDEOS, ETC.

Figures and tables are usually allowed to "float", which means that their placement is determined by LATEX, while the document is being typeset.

Use the figure environment for a figure, the table

Test Figure

 ${
m FIG.}$ 1. A figure caption. The figure captions are automatically numbered.

environment for a table. In each case, use the \caption command within to give the text of the figure or table caption along with the \label command to provide a key for referring to this figure or table. The typical content of a figure is an image of some kind; that of a table is an alignment.

Insert an image using either the graphics or graphix packages, which define the \includegraphics{#1} command. (The two packages differ in respect of the optional arguments used to specify the orientation, scaling, and translation of the image.) To create an alignment, use the tabular environment.

The best place to locate the figure or table environment is immediately following its first reference in text; this sample document illustrates this practice for Fig. 1, which shows a figure that is small enough to fit in a single column.

In exceptional cases, you will need to move the float earlier in the document, as was done with Table II: LATEX's float placement algorithms need to know about a full-page-width float earlier.

Fig. 2 has content that is too wide for a single column, so the figure* environment has been used.

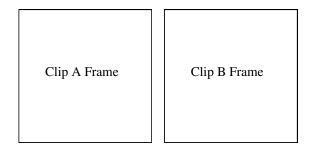
The content of a table is typically a tabular environment, giving rows of type in aligned columns. Column entries separated by &'s, and each row ends with \\. The required argument for the tabular environment specifies how data are aligned in the columns. For instance, entries may be centered, left-justified, right-justified, aligned on a decimal point. Extra column-spacing may be be specified as well, although REVT_FX 4 sets this spacing so that the columns fill the width of the table. Horizontal rules are typeset using the \hline command. The doubled (or Scotch) rules that appear at the top and bottom of a table can be achieved enclosing the tabular environment within a ruledtabular environment. Rows whose columns span multiple columns can be typeset using the \multicolumn{#1}{#2}{#3} command (for example, see the first row of Table II).

Tables I, II, III, and IV show various effects. A table that fits in a single column employs the table environ-

TABLE I. A table that fits into a single column of a two-column layout. Note that REVTEX 4 adjusts the intercolumn spacing so that the table fills the entire width of the column. Table captions are numbered automatically. This table illustrates left-, center-, decimal- and right-aligned columns, along with the use of the ruledtabular environment which sets the Scotch (double) rules above and below the alignment, per APS style.

Left ^a	Centered ^b	Decimal	Right
1	2	3.001	4
10	20	30	40
100	200	300.0	400

^a Note a.



Video 1. Students explain their initial idea about Newton's third law to a teaching assistant. Clip (a): same force. Clip (b): move backwards.

ment. Table II is a wide table, set with the table* environment. Long tables may need to break across pages. The most straightforward way to accomplish this is to specify the [H] float placement on the table or table* environment. However, the LATEX $2_{\mathcal{E}}$ package longtable allows headers and footers to be specified for each page of the table. A simple example of the use of longtable can be found in the file summary.tex that is included with the REVTEX 4 distribution.

There are two methods for setting footnotes within a table (these footnotes will be displayed directly below the table rather than at the bottom of the page or in the bibliography). The easiest and preferred method is just to use the \footnote{#1} command. This will automatically enumerate the footnotes with lowercase roman letters. However, it is sometimes necessary to have multiple entries in the table share the same footnote. In this case, there is no choice but to manually create the footnotes using \footnotemark[#1] and \footnotetext[#1]{#2}. #1 is a numeric value. Each time the same value for #1 is used, the same mark is produced in the table. The \footnotetext[#1]{#2} commands are placed after the tabular environment. Examine the LATEX source and output for Tables I and IV for examples.

Video 1 illustrates several features new with REVTEX4.2, starting with the video environment, which is in the same category with figure and table. The \setfloatlink command causes the title of the video to be a hyperlink to the indicated URL; it may be used with any environment that takes the \caption command. The \href command has the same significance as it does in the context of the hyperref package: the second argument is a piece of text to be typeset in your document; the first is its hyperlink, a URL.

Physical Review style requires that the initial citation of figures or tables be in numerical order in text, so don't cite Fig. 2 until Fig. 1 has been cited.

ACKNOWLEDGMENTS

We wish to acknowledge the support of the author community in using REVTEX, offering suggestions and encouragement, testing new versions,

^b Note b.

Wide Test Figure

FIG. 2. Use the figure* environment to get a wide figure that spans the page in twocolumn formatting.

TABLE II. This is a wide table that spans the full page width in a two-column layout. It is formatted using the table* environment. It also demonstates the use of \multicolumn in rows with entries that span more than one column.

	D	$egin{array}{c} 1 \ 4h \end{array}$	\overline{L}	O_{4h}^5
Ion	1st alternative	2nd alternative	lst alternative	2nd alternative
K	(2e) + (2f)	(4i)	(2c) + (2d)	(4f)
Mn	$(2g)^{\mathrm{a}}$	(a) + (b) + (c) + (d)	(4e)	(2a) + (2b)
Cl	(a) + (b) + (c) + (d)	$(2g)^{\mathrm{a}}$	$(4e)^{a}$	
He	$(8r)^{\mathrm{a}}$	$(4j)^{\mathrm{a}}$	$(4g)^{\mathrm{a}}$	
Ag		$(4k)^{\mathrm{a}}$		$(4h)^{\mathrm{a}}$

^a The z parameter of these positions is $z \sim \frac{1}{4}$.

Appendix A: Appendixes

To start the appendixes, use the \appendix command. This signals that all following section commands refer to appendixes instead of regular sections. Therefore, the \appendix command should be used only once—to setup the section commands to act as appendixes. Thereafter normal section commands are used. The heading for a section can be left empty. For example,

\appendix \section{}

will produce an appendix heading that says "APPENDIX A" and

\appendix \section{Background}

will produce an appendix heading that says "APPENDIX A: BACKGROUND" (note that the colon is set automatically).

TABLE III. Numbers in columns Three—Five are aligned with the "d" column specifier (requires the dcolumn package). Nonnumeric entries (those entries without a ".") in a "d" column are aligned on the decimal point. Use the "D" specifier for more complex layouts.

One	Two	Three	Four	Five
one	two	three	four	five
$_{\mathrm{He}}$	2	2.77234	45672.	0.69
C^{a}	$C_{\rm p}$	12537.64	37.66345	86.37

^a Some tables require footnotes.

If there is only one appendix, then the letter "A" should not appear. This is suppressed by using the star version of the appendix command (\appendix* in the place of \appendix).

Appendix B: A little more on appendixes

Observe that this appendix was started by using

\section{A little more on appendixes}

TABLE IV. A table with numerous columns that still fits into a single column. Here, several entries share the same footnote. Inspect the LATEX input for this table to see exactly how it is done.

	r_c (Å)	r_0 (Å)	κr_0		r_c (Å)	r_0 (Å)	κr_0
Cu	0.800	14.10	2.550	Sna	0.680	1.870	3.700
Ag	0.990	15.90	2.710	$\mathrm{Pb^{b}}$	0.450	1.930	3.760
Au	1.150	15.90	2.710	Ca^{c}	0.750	2.170	3.560
Mg	0.490	17.60	3.200	$\mathrm{Sr^d}$	0.900	2.370	3.720
Zn	0.300	15.20	2.970	Li^{b}	0.380	1.730	2.830
Cd	0.530	17.10	3.160	Na^{e}	0.760	2.110	3.120
$_{\mathrm{Hg}}$	0.550	17.80	3.220	K^{e}	1.120	2.620	3.480
Al	0.230	15.80	3.240	Rb^{c}	1.330	2.800	3.590
Ga	0.310	16.70	3.330	Cs^d	1.420	3.030	3.740
In	0.460	18.40	3.500	$\mathrm{Ba^e}$	0.960	2.460	3.780
Tl	0.480	18.90	3.550				

^a Here's the first, from Ref. 2.

^b Some tables need more than one footnote.

 $^{^{\}rm b}$ Here's the second.

^c Here's the third.

^d Here's the fourth.

^e And etc.

Note the equation number in an appendix:

$$E = mc^2. (B1)$$

1. A subsection in an appendix

You can use a subsection or subsubsection in an appendix. Note the numbering: we are now in Ap-

pendix B1.

Note the equation numbers in this appendix, produced with the subequations environment:

$$E = mc,$$
 (B2a)

$$E = mc^2, (B2b)$$

$$E \gtrsim mc^3$$
. (B2c)

They turn out to be Eqs. (B2a), (B2b), and (B2c).

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- [2] See the explanation of time travel in R. P. Feynman, Phys. Rev. 94, 262 (1954); The classical relativistic treatment of A. Einstein, Yu. Podolsky, and N. Rosen (EPR), ibid. 47, 777 (1935) is a relative classic
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