2D Ising Model with MCMC: Group B

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(Dated: March 23, 2024)

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

A. 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:

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

Here, J denotes the coupling constant, B represents the external magnetic field, and the terms $\sum_{\langle ij \rangle}$ and $\sum_{i \in \Lambda}$ 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 $-B \sum_{i \in \Lambda} \sigma_i$ 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:

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

Here, $|\Lambda|$ represents the total number of lattice sites.

Attach some snapshots of low temperature, negative magnetic field; low temperature, positive magnetic field.

B. 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 eachdirected 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.

II. RESULTS AND DISCUSSION

A. Configuration and Burn-In

We've developed an algorithm for determining the appropriate number of burn-in steps for a given Ising model simulation. The primary objective of this algorithm is computational efficiency. If the absolute difference between these two values falls below the error threshold, we backtrack by 25% of the array's length. We then compute the absolute difference of this value with $h1$ and compare it against the error. If it exceeds the error, we move forward by 12.5%; conversely, if it falls below the

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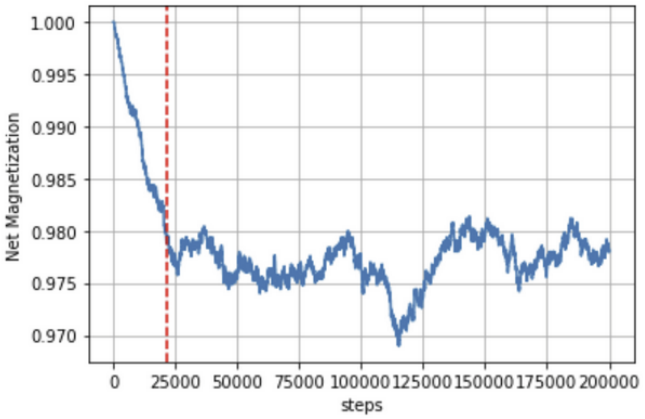


FIG. 1. Burn-in, starting with all up spins

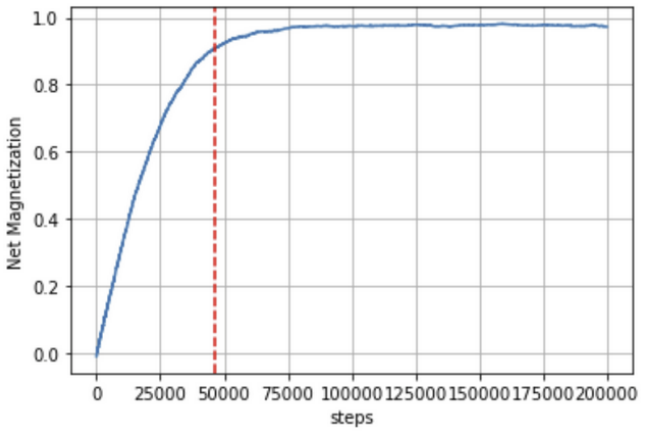


FIG. 2. Burn-in, starting with random spins

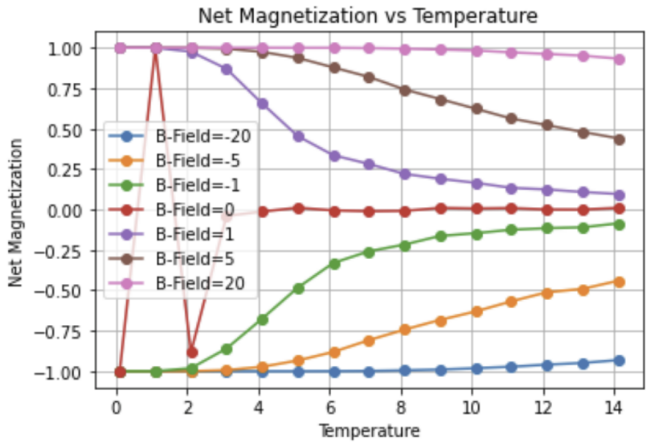


FIG. 3. M vs T for fixed B

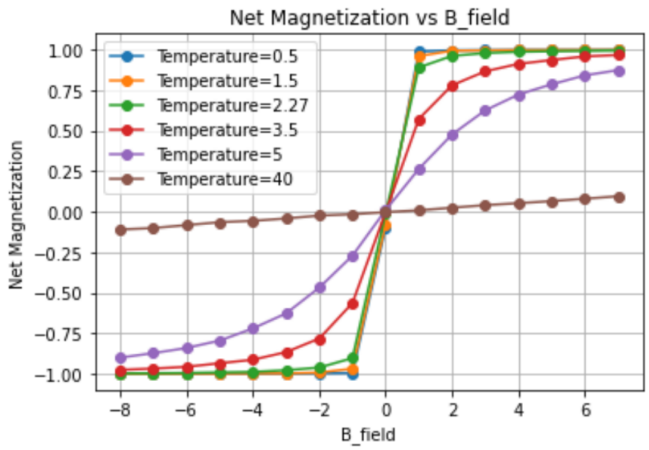


FIG. 4. M vs B for fixed T

error, we backtrack by 12.5%. It's worth noting that the percentage values we use for moving back and forth are based on the inverse powers of two, ensuring a geometrically decreasing step size. For instance, we move back by 50% (1/2) of the array's length, then by 25% (1/4), and subsequently by 12.5% (1/8), and so forth. This geometric progression allows for a systematic exploration of the magnetization history, optimizing the search for the appropriate burn-in steps.

In the scenario where the first absolute difference yields a value greater than the error, we transition to a mean sampling method. Here, we randomly sample a subset of points (typically ranging from 5 to 20) from the magnetization history. Subsequently, we compute the mean of this sample and conduct a linear search from the beginning of the magnetization history. We continue this search until we locate a value below or above the mean, depending on whether the history is converging downwards or upwards.

One notable advantage of this algorithm is its reliability in yielding results, albeit with a caveat. In instances where the magnetization history exhibits significant noise, the error-based method often fails, defaulting instead to mean sampling. However, it's worth noting that this may not always produce accurate results.

B. 1D Scans of Magnetization vs Temperature

When plotting magnetization vs temperature for constant magnetic field (figure 3), we can observe that when the magnetic field (B) is zero, the net magnetization undergoes a rather sudden transition to an all-random state. Conversely, if there is any non-zero B field, the transition is much slower, but the net magnetization eventually converges to around zero, albeit at a higher temperature. These transitions to an all-random state represent a second-order phase transition of the material.

Plotting magnetization vs external field for fixed temperature (figure 4), we observed a discontinuity at about $B = 0$ for low temperatures, corresponding to a first-order phase transition. For higher temperatures, we noticed that the net magnetization flattens out and converges to around zero, regardless of the magnetic field.

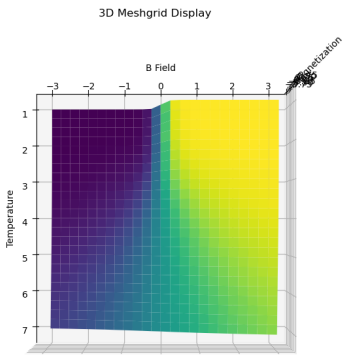


FIG. 5. Phase Diagram

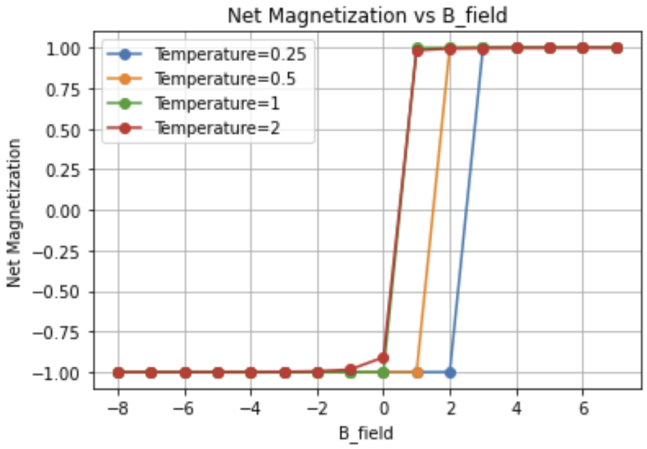


FIG. 6. Enter Caption

C. Phase Diagram, Metastable States, and Hysteresis

The inherent stability of aligned spins gives rise to metastable states - states that are local potential minima (resistant to perturbation and thus stable), but not global minima (i.e. not the least possible energy). Here, if a low-temperature lattice begins in an all-up or all-down state, it is able to resist an external field in the opposite direction for some time, before eventually becoming overpowered by a strong-enough field. This dependence upon the initial state is called hysteresis, and can give rise to lattices that have a sort of "memory" of their recent states. Systems that exhibit hysteresis are hard to solve analytically due to this dependence of the current state on prior states. We have graphed some of these hysteresis curves, where the phase transition from down to up or up to down spin depends on which way the aligned spins began in (figures 6 and 7).

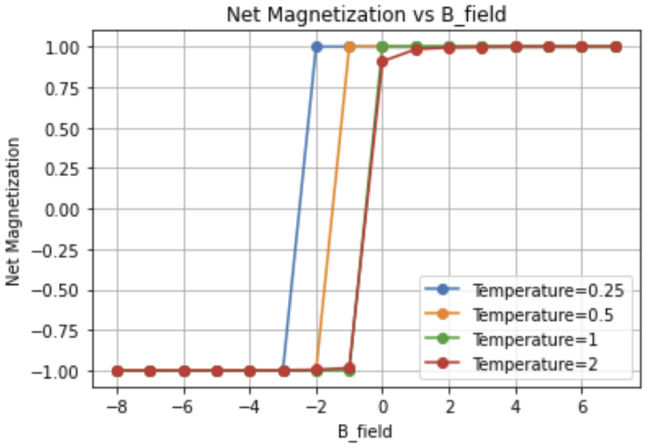


FIG. 7. Enter Caption

III. PROFILING AND OPTIMIZATION

To make the code run in a reasonable amount of time, we used a combination of high code separation, Numba, and Scalene. In general, to make the most use out of the tools we had, we used a functional style of programming, and separated code functionality as far as we could, trying as much as possible to ensure each function had as few responsibilities as possible (preferably exactly 1). This way, when we optimized, we could fast-track development by limiting Numba applications only the code most critical to performance, reducing the need to untangle the strict typing and compilation requirements to get Numba working on a larger scale. It also helped us to profile code, as while the tool we used, Scalene, can profile individual lines of code, it is much better at profiling entire functions. Numba is a set of C libraries with a front-end accessible via Python. This allows developers to use highly performant C code from within much easier-to-use Python. It works best when breaking down loops and iterations, as well as large matrix operations, which Python struggles to do at speed by itself. Lastly, we used Scalene, a profiling tool that tracks time spent per line and per function in the code, including the proportions of time spent by the processor running in Python, native bytecode, and C. It also tracks memory and GPU usage. With the combination of these three, we were able to track down the fact that our performance bottleneck lay in the ΔE calculation during simulation steps when determining whether or not to flip a cell's spin. Figure 8 is a screen capture of our code's performance running a low-resolution pass.

This sample document demonstrates proper use of REVTEX 4.2 (and LATEX 2_ε) in mansucripts 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,

FIG. 8. Scalene profile of our simulation

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 commands. 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 6. (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: `\cite { [ {`*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. REVTEX 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 `\bibitem` commands (including extra markup information via `\bibinfo` and `\bibfield` commands). If not using BibTEX, you will have to create the `thebibiliography` environment and its `\bibitem` 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.*

IV. MATH AND EQUATIONS

Inline math may be typeset using the `$` delimiters. Bold math symbols may be achieved using the `bm` package and the `\bm{#1}` command it supplies. For instance, a bold α can be typeset as `$\bm{\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, `$\mathbb{R}$` gives $\mathbb{R}$ and `$\mathfrak{G}$` gives $\mathfrak{G}$

In LATEX 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*:

$$\chi_+(p) \lesssim [2|\mathbf{p}|(|\mathbf{p}|+p_z)]^{-1/2} \begin{pmatrix} |\mathbf{p}|+p_z \\ px+ip_y \end{pmatrix}, \quad (3)$$

$$\left\{ \mathbb{1}234567890abc123\alpha\beta\gamma\delta1234556\alpha\beta \frac{1\sum_b^a}{A^2} \right\}. \quad (4)$$

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:

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

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:

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

A. Multiline equations

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

$$\begin{aligned}\mathcal{M} =& ig_Z^2(4E_1E_2)^{1/2}(l_i^2)^{-1}\delta_{\sigma_1,-\sigma_2}(g^e_{\sigma_2})^2\chi_{-\sigma_2}(p_2) \\ & \times[\epsilon_j l_i \epsilon_i]_{\sigma_1}\chi_{\sigma_1}(p_1),\end{aligned} \tag{6}$$

$$\begin{aligned}\sum|M_g^{\rm viol}|^2 =& \, g_S^{2n-4}(Q^2)\ N^{n-2}(N^2-1) \\ & \times\left(\sum_{i<j}\right)\sum_{\rm perm}\frac{1}{S_{12}}\frac{1}{S_{12}}\sum_\tau c_\tau^f \ .\end{aligned} \tag{7}$$

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:

$$\begin{aligned}\sum|M_g^{\rm viol}|^2 =& \, g_S^{2n-4}(Q^2)\ N^{n-2}(N^2-1) \\ & \times\left(\sum_{i<j}\right)\left(\sum_{\rm perm}\frac{1}{S_{12}S_{23}S_{n1}}\right)\frac{1}{S_{12}} \ .\end{aligned}$$

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

$$g^+g^+ \to g^+g^+g^+g^+ \dots \ , \quad q^+q^+ \to q^+g^+g^+ \dots \ . \tag{2.6′}$$

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.

$$\begin{aligned}\mathcal{M} =& ig_Z^2(4E_1E_2)^{1/2}(l_i^2)^{-1}(g^e_{\sigma_2})^2\chi_{-\sigma_2}(p_2) \\ & \times[\epsilon_i]_{\sigma_1}\chi_{\sigma_1}(p_1).\end{aligned} \tag{8a}$$

$$\left\{abc123456abcdef\alpha\beta\gamma\delta1234556\alpha\beta\frac{1\sum_b^a}{A^2}\right\}, \tag{8b}$$

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:

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

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.)

V. CROSS-REFERENCING

REVTEX 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 III on page 3, Table I, and Fig. 9.

VI. 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` 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. 9, 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. 10 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 REVTeX 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` environment. 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_ε 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

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.
[b] Note b.

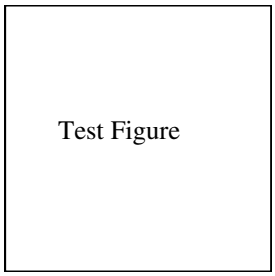


FIG. 9. A figure caption. The figure captions are automatically numbered.

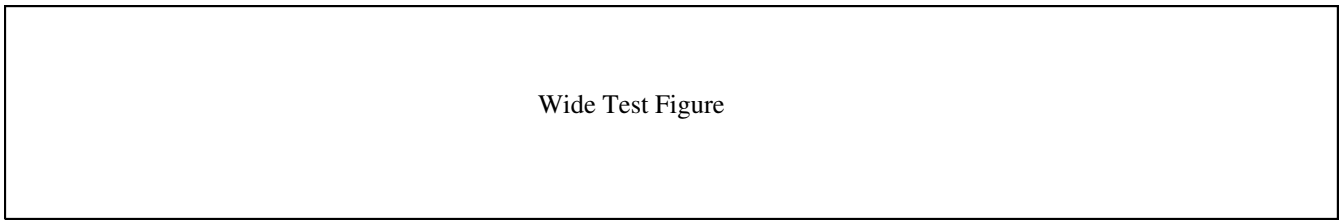
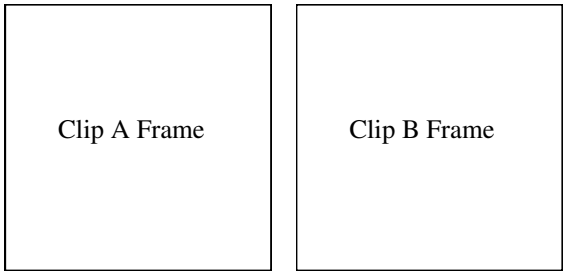


FIG. 10. Use the figure* environment to get a wide figure that spans the page in `twocolumn` formatting.

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^1_{4h}		D^5_{4h}	
Ion	1st alternative	2nd alternative	lst alternative	2nd alternative
K	$(2e)+(2f)$	$(4i)$	$(2c)+(2d)$	$(4f)$
Mn	$(2g)$[a]	$(a)+(b)+(c)+(d)$	$(4e)$	$(2a)+(2b)$
Cl	$(a)+(b)+(c)+(d)$	$(2g)$[a]	$(4e)$[a]	
He	$(8r)$[a]	$(4j)$[a]	$(4g)$[a]	
Ag		$(4k)$[a]		$(4h)$[a]

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



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

Physical Review style requires that the initial citation of figures or tables be in numerical order in text, so don't cite Fig. 10 until Fig. 9 has been cited.

ACKNOWLEDGMENTS

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

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.

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
He	2	2.77234	45672.	0.69
C[a]	C[b]	12537.64	37.66345	86.37

[a] Some tables require footnotes.
[b] Some tables need more than one footnote.

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	Sn[a]	0.680	1.870	3.700
Ag	0.990	15.90	2.710	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	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
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	Ba[e]	0.960	2.460	3.780
Tl	0.480	18.90	3.550				

[a] Here's the first, from Ref. 2.
[b] Here's the second.
[c] Here's the third.
[d] Here's the fourth.
[e] And etc.

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).

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}
```

Note the equation number in an appendix:

$$E = mc^2. \tag{B1}$$

1. A subsection in an appendix

You can use a subsection or subsubsection in an appendix. Note the numbering: we are now in Appendix B 1.

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

$$E = mc, \tag{B2a}$$
$$E = mc^2, \tag{B2b}$$
$$E \gtrsim mc^3. \tag{B2c}$$

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

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