

Quantum Simulation of the H_2 Molecule*

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ABSTRACT

Our project focuses on simulating the behavior and energy of the H_2 molecule in various quantum scenarios. Through this exploration, we've captured key insights into the ground state energy and effects of different perturbations.

Simulation and Ground State	<ul style="list-style-type: none">• H_2 Molecule: Simulated the H_2 molecule using a quantum approach.• VQE (Variational Quantum Eigensolver): Determined the ground state energy of the H_2 molecule.
Trotterisation and Perturbation	<ul style="list-style-type: none">• Trotterisation: Applied the Trotterisation method to see the changes in energy due to a perturbation.• Time-Dependent Perturbation: Introduced a time-dependent perturbation to study its effects.
Application of Magnetic Field	<ul style="list-style-type: none">• Magnetic Field Orientation: Applied a magnetic field that transitions from the X to the Z axis.• Analysis: Observed and documented the effect of the changing magnetic field on the ground state energy of the H_2 molecule.

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

This sample document demonstrates proper use of REVTeX 4.2 (and L^AT_EX 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 T_EX 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 T_EX 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 ?? . (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... },`

* A footnote to the article title

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. [?] and the two under Ref. [?]). (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 L^AT_EX 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. [?]). 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. [?]. 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 BibT_EX 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[?]. Author-year citations are used when the journal is RMP. To give a textual citation, use `\onlinecite{#1}`: Refs. [?]. By default, the `natbib` package automatically sorts your citations into numerical order and “compresses” runs of three or more consecutive numerical citations. REV_TE_X 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 [? ? ?

?, and once again in different order (Refs. [? ? ? ? ? ?]). Note that the citations were both compressed and sorted. Furthermore, 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 BibT_EX. REV_TE_X 4.2 includes BibT_EX 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 `report.bbl` file and specifies which bibliographic databases are to be used by BibT_EX (one of these should be by arXiv convention `report.bib`). Running BibT_EX (via `bibtex report`) after the first pass of L^AT_EX produces the file `report.bbl` which contains the automatically formatted `\bibitem` commands (including extra markup information via `\bibinfo` and `\bibfield` commands). If not using BibT_EX, you will have to create the `thebibliography` 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 `report.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[?]; 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 BibT_EX every time you change any of your document’s footnotes.*

II. 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 α . 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*:

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

$$\left\{ 1234567890abc123\alpha\beta\gamma\delta1234556\alpha\beta\frac{1\sum_b^a}{A^2} \right\}. \quad (2)$$

Note the open one in Eq. (??).

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:

$$\left\{ ab12345678abc123456abcde\alpha\beta\gamma\delta1234556\alpha\beta\frac{1\sum_b^a}{A^2} \right\}. \quad (3)$$

When the `\label{#1}` command is used [cf. input for Eq. (??)], 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:

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

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:

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

$$\sum |M_g^{\text{viol}}|^2 = g_S^{2n-4} (Q^2) N^{n-2} (N^2 - 1) \times \left(\sum_{i < j} \right) \sum_{\text{perm}} \frac{1}{S_{12}} \frac{1}{S_{12}} \sum_{\tau} c_{\tau}^f. \quad (5)$$

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 `\tag{#1}` command, where `#1` is the desired equation number. For example, to get an equation number of (??),

$$g^+g^+ \rightarrow g^+g^+g^+g^+ \dots, \quad q^+q^+ \rightarrow q^+g^+g^+ \dots. \quad (2.6')$$

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 \LaTeX ; 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. (??) and (??) 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.

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

$$\left\{ abc123456abcde\alpha\beta\gamma\delta1234556\alpha\beta\frac{1\sum_b^a}{A^2} \right\}, \quad (6b)$$

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. (??).

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:

$$\mathcal{R}^{(d)} = g_{\sigma_2}^e \left(\frac{[\Gamma^Z(3, 21)]_{\sigma_1}}{Q_{12}^2 - M_W^2} + \frac{[\Gamma^Z(13, 2)]_{\sigma_1}}{Q_{13}^2 - M_W^2} \right) + x_W Q_e \left(\frac{[\Gamma^\gamma(3, 21)]_{\sigma_1}}{Q_{12}^2 - M_W^2} + \frac{[\Gamma^\gamma(13, 2)]_{\sigma_1}}{Q_{13}^2 - M_W^2} \right). \quad (7)$$

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.)

III. 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 ?? on page ??, Table ??, and Fig. ??.

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

Figures and tables are usually allowed to “float”, which means that their placement is determined by L^AT_EX, 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 `graphicx` packages, which define the `\includegraphics{#1}` com-

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.

mand. (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. ??, 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 ??: L^AT_EX’s float placement algorithms need to know about a full-page-width float earlier.

Fig. ?? 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 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 ??).

Tables ??, ??, ??, and ?? show various effects. A table that fits in a single column employs the `table` environment. Table ?? 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 L^AT_EX 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 let-

FIG. 1. A figure caption. The figure captions are automatically numbered.

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 demonstrates the use of `\multicolumn` in rows with entries that span more than one column.

Ion	D_{4h}^1		D_{4h}^5	
	1st alternative	2nd alternative	1st 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.

ters. 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 L^AT_EX source and output for Tables ?? and ?? for examples.

Video ?? illustrates several features new with REV_TE_X4.2, 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. ?? until Fig. ?? has been cited.

TABLE III. Numbers in columns Three–Five are aligned with the “d” column specifier (requires the `dcolumn` package). Non-numeric 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.

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

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{}
```

TABLE IV. A table with numerous columns that still fits into a single column. Here, several entries share the same footnote. Inspect the L^AT_EX 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	Si ^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. ? .

^b Here’s the second.

^c Here’s the third.

^d Here’s the fourth.

^e And etc.

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 ??.

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. (??), (??), and (??).