

Quantum Simulation of the H_2 Molecule*

Robert Negrin, Saleh Naghdi, Yarin Heffes, and Manvi Agrawal
*University of California
Los Angeles, California*
(Dated: October 24, 2023)

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. INITIAL SIMULATION AND GROUND STATE H_2 MOLECULE

We utilized Qiskit's 'PySCFDriver' to define the H_2 molecule. The electronic structure of the molecule is initially described in terms of fermionic creation and annihilation operators.

Now, transform this fermionic Hamiltonian into a qubit (spin) Hamiltonian suitable for quantum computation. For our simulation we have used Jordan-Wigner Transformation which provides a direct mapping of fermions to qubits. Bravyi-Kitaev Transformation is another more efficient mapping especially for systems with local interactions, but its more complex in form.

A. Second-level heading: Formatting

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.

B. 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 BibTeX 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*:

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

$$\left\{ 1234567890abc123\alpha\beta\gamma\delta123456\alpha\beta\frac{1\sum_b^a}{A^2} \right\}. \quad (2)$$

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:

$$\left\{ ab12345678abc123456abcdef\alpha\beta\gamma\delta123456\alpha\beta\frac{1\sum_b^a}{A^2} \right\}. \quad (3)$$

* A footnote to the article title

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:

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

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

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:

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

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 (??),

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

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 \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. (??) 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.

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

$$\left\{ abc123456abcdef\alpha\beta\gamma\delta1234556\alpha\beta\frac{1\sum_b^a}{A^2} \right\}, \quad (6b)$$

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}` 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. ??, 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` environ-

TABLE I. A table that fits into a single column of a two-column layout. Note that REV_TE_X 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.

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, 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 REV_TE_X 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 REV_TE_X 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 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

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 $z \sim \frac{1}{4}$.

`\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.

ACKNOWLEDGMENTS

We wish to acknowledge the support of the author community in using REVTeX, 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 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.

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}
```

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.

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 ??.

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