

QuantumBench: A Benchmark for Quantum Problem Solving

Anonymous submission

Abstract

Large language models are now integrated into many scientific workflows, accelerating data analysis, hypothesis generation, and design space exploration. In parallel with this growth, there is a growing need to carefully evaluate whether models accurately capture domain-specific knowledge and notation, since general-purpose benchmarks rarely reflect these requirements. This gap is especially clear in quantum science, which features non-intuitive phenomena and requires advanced mathematics. In this study, we introduce QuantumBench, a benchmark for the quantum domain that systematically examine how well LLMs understand and can be applied to this non-intuitive field. Using publicly available materials, we compiled approximately 800 questions with their answers spanning nine areas related to quantum science and organized them into an eight-option multiple-choice dataset. With this benchmark, we evaluate several existing LLMs and analyze their performance in the quantum domain, including sensitivity to changes in question format. QuantumBench is the first LLM evaluation dataset built for the quantum domain, and it is intended to guide the effective use of LLMs in quantum research.

Keywords: Large Language Models, Benchmarking, Question Answering, Quantum Science

1. Introduction

Recent advances in large language models (LLMs) are reshaping scientific research activities. Beyond information gathering, paper summarization and manuscript drafting, LLMs are now used for hypothesis generation and experimental design. Furthermore, recent studies are beginning to demonstrate the utility of research-agent systems for end-to-end research workflows, including AI Scientist ([Lu et al., 2024](#); [Yamada et al., 2025](#)) and Agent Laboratory ([Schmidgall et al., 2025](#)). These developments indicate a plausible path toward greater automation of the research pipeline and raise the prospect of AI-enabled scientific discoveries.

For example, in quantum science, LLMs are applied to tasks ranging from code generation to experimental design. The Qiskit Code Assistant ([Dupuis et al., 2024](#)) can generate code for quantum programming with the Qiskit library ([Javadi-Abhari et al., 2024](#)), and is integrated into the IBM Quantum platform. Similarly, El Agente Q ([Zou et al., 2025](#)) autonomously conducts quantum chemistry calculations by orchestrating more than twenty domain-specific agents under LLM supervision. With natural-language instructions alone, users can prepare input files and execute computations, enabling non-specialists to perform advanced quantum chemistry simulations. In addition, the agent-based AI framework called k-agents automates quantum-computing experiments by planning, executing, and analyzing them using LLMs ([Cao et al., 2025](#)).

However, the performance of LLMs on scientific tasks has not yet been sufficiently validated. LLMs can generate plans with serious errors and inconsistencies, such as fabricated references or datasets, as well as proposals for physically infeasible experimental conditions ([Eger et al., 2025](#)). In

quantum many-body physics, for example, LLMs perform well on prescribed computational procedures but show limited ability to incorporate physical context when planning experiments ([Pan et al., 2025](#)). These observations imply that LLMs do not yet possess robust, domain-specific scientific reasoning, underscoring the need to assess whether they genuinely acquire domain knowledge.

In this work, we focus on quantum science, a domain marked by non-intuitive phenomena and advanced mathematical structures, where existing general-purpose benchmarks are likely insufficient to evaluate LLM performance adequately. To address this challenge, we construct QuantumBench, a benchmark dataset that systematically assesses how well LLMs understand and can be applied to quantum science. Using publicly available resources such as MIT OpenCourseWare ([Massachusetts Institute of Technology](#)), TU Delft OpenCourseWare ([Delft University of Technology](#)), and LibreTexts ([LibreTexts](#)), we have selected fifteen courses and textbooks related to quantum science and collected the corresponding lecture notes, exercises, and assignments. From these materials, question-answer pairs have been created, and encoded as eight-option multiple-choice questions with plausible but incorrect options alongside the correct answer. QuantumBench comprises approximately 800 undergraduate-level question-answer pairs across nine quantum-related subfields.

QuantumBench enables comprehensive, comparative evaluation of existing LLMs in the quantum domain. We quantify LLM performance on quantum tasks, including sensitivity to variation in question format and wording. Beyond quantum science, the benchmark highlights the need for further improvements in the use of LLMs across scientific fields and helps accelerate the development of AI for scientific research.

2. Related Work

Various general-purpose benchmarks exist. For example, The Massive Multitask Language Understanding (MMLU) benchmark (Hendrycks et al., 2020) is a widely used benchmark of the general capabilities of LLMs across academic and professional domains. It comprises multiple-choice questions from 57 subjects, including elementary mathematics and computer science, and assesses broad knowledge relevant to research. MMLU-Pro (Wang et al., 2024) extends MMLU by increasing the number of answer choices to ten to raise reasoning difficulty. For advanced evaluations, GPQA (Rein et al., 2024) is proposed as a representative benchmark targeting PhD-level subjects with expert-authored, high-quality problems that are not answerable through simple search or shallow reasoning, making it a standard for assessing doctoral-level competence. More recently, Humanity’s Last Exam (Phan et al., 2025) spans dozens of fields across mathematics, the humanities, and the natural sciences, and includes 3,000 ultra-challenging problems that demand deep reasoning and advanced expertise beyond data lookup.

Numerous domain-specific benchmark datasets have also been proposed. For mathematics, MATH (Hendrycks et al., 2021) contains about 12,500 problems drawn from competitive contests in the United States, spanning algebra, number theory, geometry, probability, and combinatorics. Unlike general benchmarks such as MMLU and GPQA, which primarily use multiple-choice formats, MATH employs short-answer, free-response questions without predefined options, thereby evaluating precise mathematical reasoning and solution derivation. In the biomedical domain, PubMedQA (Jin et al., 2019) is a representative benchmark, containing approximately 1,000 questions in the form of “Yes/No/Maybe,” created based on academic questions from papers published in PubMed. PubMedQA is widely used to evaluate large language models’ ability to understand and interpret medical contexts, thereby facilitating advancements in biomedical research and drug discovery. Collectively, such domain-specific benchmarks probe specialized abilities and sensitivity to the representations and conventions of each field that general-purpose evaluations do not capture, enabling more valid assessments of model performance in real-world settings.

In contrast, benchmark datasets specialized for the quantum domain remain limited. Within GPQA, only 64 items cover quantum mechanics. More recently, CritPt (Zhu et al., 2025) was introduced to test whether models can perform advanced scientific reasoning required in frontier physics; it comprises 71 challenges with 190 intermediate reason-

ing checkpoints, including 15 questions in quantum information science and technology. While these resources are valuable for assessing capabilities across science and physics, they are insufficient for comprehensive benchmarking of model ability in quantum science.

For quantum-specific evaluation, major efforts focus on coding skill for quantum programming, with benchmarks such as QiskitHumanEval (Vishwakarma et al., 2024) and QCoder Benchmark (Mikuriya et al., 2025). As a corpus of question–answer pairs, QuantumLLMInstruct (QLMMI) (Kashani, 2024) includes 500,000 items. However, since QLMMI was generated entirely by LLMs, and designed for fine-tuning rather than rigorous evaluation, it does not serve as an adequate benchmark for assessing model performance. Human-authored datasets such as MMLU and GPQA remain important for advancing applications. In this study, we construct a benchmark from publicly available resources by collecting undergraduate-level questions authored by domain experts, thereby providing an evaluation framework for knowledge understanding and reasoning in the quantum domain.

3. QuantumBench

In this section, we outline the construction procedure of QuantumBench and present an overview of the dataset.

3.1. Dataset Construction

We selected 15 quantum science-related online courses and teaching materials from MIT OpenCourseWare, TU Delft OpenCourseWare, and LibreTexts. These sources include assignments and examinations together with instructor-provided solutions. From these materials, we chose 769 questions for which the question–answer mapping was unambiguous and the solution was uniquely determined. Table 1 summarizes the course titles, subject areas, and the number of collected items.

Next, we preprocessed the collected question statements. To ensure that each question can be understood and solved in isolation, we manually augmented the texts with missing information, including implicit notation and unstated definitions, with assistance from an LLM (gpt-oss-120b (Agarwal et al., 2025)). We also used the LLM to flag ambiguities or omissions and to check internal consistency and completeness. For each problem, we created seven plausible but incorrect options in addition to the correct answer. These options were human-curated and cover not only simple mistakes, such as sign errors, but also responses reflecting

Platform	Lecture Titles	Domain	Number of Problems
MIT OCW	Computational Quantum Mechanics of Molecular and Extended Systems	Quantum Chemistry	2
MIT OCW	Introduction to Applied Nuclear Physics	Nuclear Physics	38
MIT OCW	Introductory Quantum Mechanics I	Quantum Mechanics	5
MIT OCW	Optics (2014)	Optics	49
MIT OCW	Optics (2009)	Optics	122
MIT OCW	Quantum Computation	Quantum Computation	43
MIT OCW	Quantum Optical Communication	Photonics	118
MIT OCW	Quantum Physics I	Quantum Mechanics	130
MIT OCW	Relativistic Quantum Field Theory I	Quantum Field Theory	81
MIT OCW	Relativistic Quantum Field Theory II	Quantum Field Theory	21
MIT OCW	Relativistic Quantum Field Theory III	Quantum Field Theory	8
MIT OCW	String Theory and Holographic Duality	String Theory	23
MIT OCW	String Theory	String Theory	17
TUD OCW	Quantum Information Processing	Quantum Computation	19
LibreTexts	Physical Chemistry I, Quantum Mechanics	Quantum Chemistry	93

Table 1: The titles of the lectures used as data sources, their corresponding academic fields, and the number of questions collected

	Algebraic Calculation	Numerical Calculation	Conceptual Understanding	Total
Quantum Mechanics	177	21	14	212
Quantum Computation	54	1	5	60
Quantum Chemistry	16	64	6	86
Quantum Field Theory	104	1	2	107
Photonics	54	1	2	57
Mathematics	37	0	0	37
Optics	101	41	15	157
Nuclear Physics	1	15	2	18
String Theory	31	0	2	33
Total	575	144	50	769

Table 2: Number of questions per domains

misinterpretation of the statement or mistakes arising at intermediate calculations.

Finally, some of the authors annotated each problem with one of three question types: algebraic calculation (symbolic manipulation and formula derivation), numerical calculation (computations with explicit numerical values), and conceptual understanding (knowledge- and principle-based questions without explicit calculation). We also assigned a field label to each problem. Because some courses include questions from related areas (for example, a quantum mechanics course may include a few quantum chemistry questions), we relabeled fields based on actual content to improve the quality of categorization. The category comprises nine fields in total: eight lecture-oriented fields plus an additional Mathematics category.

We also categorized all 769 problems by difficulty and expertise level. Three researchers in quantum science performed the level annotation, rating difficulty level on a five-point scale from Level 1 (trivial) to Level 5 (challenging) and expertise level on a four-point scale from Level 1 (high school) to Level 4 (PhD). It is acceptable that the annotators do not assign levels to some items because those topics were outside their areas of expertise. For each problem, the final label was the median of the three ratings. The criteria appear in Table 3 and Table 4.

	Criteria
Level 1	A problem whose correct answer can be obtained immediately
Level 2	A problem with an obvious solution that can be solved with simple calculations
Level 3	A problem whose solution comes to mind quickly but requires somewhat tedious steps
Level 4	A problem that requires some thought to discover the solution, or whose solution is obvious but involves considerably tedious steps
Level 5	A problem whose solution cannot be easily identified

Table 3: Difficulty levels and their criteria

	Criteria
Level 1	An elementary problem, non-specialists can understand the question.
Level 2	People who studied physics can understand the the question.
Level 3	Understanding requires having read technical texts in the field.
Level 4	Only experts who conduct research in that field can understand the question.

Table 4: Expertise levels and their criteria

3.2. Summary of the Dataset

Table 2 shows the number of items in the final dataset by fields. Of the 769 problems, Algebraic Calculation is the largest category, with 575 items (approximately 75% of the dataset), indicating that the collection is dominated by questions focused on symbolic and analytical derivation. By subfield, quantum mechanics accounts for the largest share, followed by optics. Several representative examples are presented in Table 5.

Figure 1 shows a t-SNE (Maaten and Hinton, 2008) projection of the question statements embedded with OpenAI’s text-embedding-3-large model. The resulting clusters align with fields, indicating clear semantic separation in the embedding space. The cluster structure is roughly organized into four groups: (i) Quantum Computation, (ii) Optics, (iii) Quantum Mechanics and related areas including Quantum Chemistry and Nuclear Physics, and (iv) Quantum Field Theory and String Theory, which require advanced algebraic calculations.

Figure 2 illustrates the distribution of difficulty and expertise level across the categories (domain and type). The overall average difficulty level is 2.68, and the average expertise level is 2.37. These

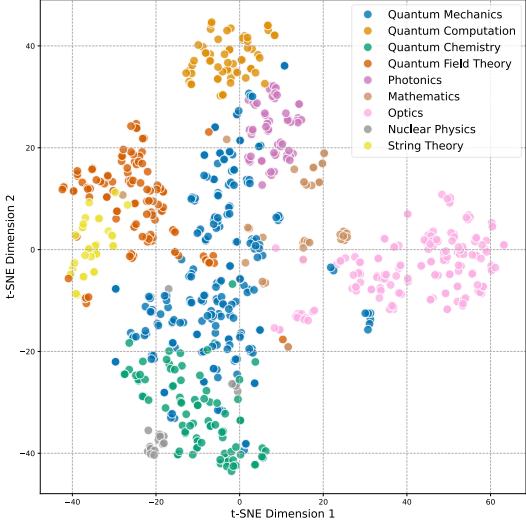


Figure 1: Visualization of QuantumBench. The questions were embedded into 3072-dimensional vectors using text-embedding-3-large, and mapped onto a two-dimensional space using t-SNE.

statistics suggest that QuantumBench primarily comprises standard-level questions typical of undergraduate education. Notably, no problems classified as difficulty level 5 (challenging) or requiring an expertise level 4 (PhD) are included. This indicates that QuantumBench serves as a benchmark to evaluate whether a model can consistently demonstrate the fundamental knowledge and reasoning abilities required for conducting research in quantum science.

Because the levels of difficulty and expertise are not uniform among domains and problem types, cross-category comparisons within a single model are not meaningful. Instead, QuantumBench should be used to evaluate model performance independently within each category, enabling fair comparisons of distinct models.

4. Experiments

We evaluated 11 OpenAI models (Brown et al., 2020; Achiam et al., 2023; Agarwal et al., 2025), 6 Meta models (Touvron et al., 2023; Dubey et al., 2024), 5 Alibaba models (Yang et al., 2025), 3 Google models (Gemini Team, 2023), 1 DeepSeek model (Guo et al., 2025), and 1 Moonshot AI model (Kimi Team, 2025). For OpenAI and Google models without public weights, inference was conducted via API; all other models were run on NVIDIA H100 GPUs using ABCI-Q. For reasoning models, we varied reasoning strength and evaluated multiple configurations. During inference, web search and external tool use were disabled to evaluate the isolate model-internal problem-solving ability. Our

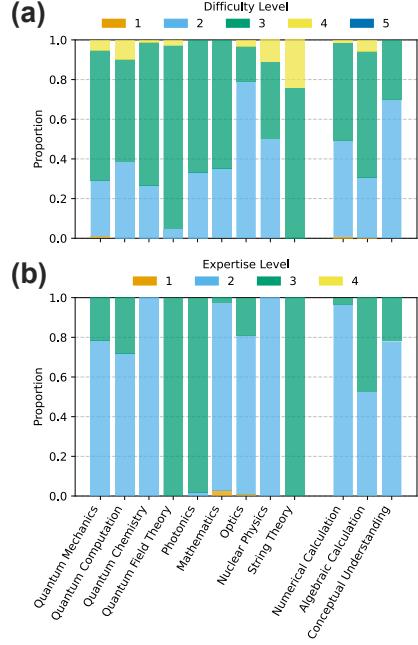


Figure 2: Distribution of difficulty and expertise levels by category. (a) Difficulty level, ranging from 1 (trivial) to 5 (challenging). (b) Expertise level, ranging from 1 (high school) to 4 (PhD). The graph shows the distribution of problems that were evaluated by at least one annotator.

benchmark data and code is available at GitHub¹.

4.1. Zero-Shot

For each problem, the model received only the question statement and answer choices, and we evaluated whether it could select the correct answer (Bowman et al., 2022). Figure 3(a) reports accuracy for all 48 model configurations on the full QuantumBench dataset. The current frontier model, GPT-5, achieved the highest performance, while open-weight models such as gpt-oss-120b and Qwen3-235B reached comparable accuracy. Most high-performing models were reasoning models. Although non-reasoning models, including Qwen3-Max and Llama4-Maverik, performed relatively well, their accuracy did not exceed 80%. These results indicate that many tasks in the quantum domain require multi-step reasoning, and that explicit mechanisms for sequential reasoning are a key determinant of performance.

Model accuracy generally increases with the number of parameters (Kaplan et al., 2020). Figure 3(b) shows the relationship between model size and accuracy, and the similar trend holds in QuantumBench. Non-reasoning models exhibit a clear performance gain as scale grows. By contrast, rea-

¹https://anonymous.4open.science/r/anon_QuantumBench-04E1/

Quantum Computation

Consider the state $\frac{1}{\sqrt{2}}(|000\rangle + |111\rangle)$. Suppose all three qubits of this state are measured in the $|+\rangle = \{\frac{1}{\sqrt{2}}(|0\rangle + |1\rangle), |-\rangle = \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle)\}$ basis. What are the possible joint outcomes of these measurements?

- | | |
|---|--|
| (A) $\frac{1}{\sqrt{2}}(-+-\rangle + +-+-\rangle)$
(B) $\frac{1}{2}(+++> + ++-\rangle + -+> + +--\rangle)$
(C) $\frac{1}{2}(+++> + ++-\rangle + -+-> + -+-\rangle)$
(D) $\frac{1}{2}(+++> + --->)$ | (E) $\frac{1}{\sqrt{2}}(-+-\rangle + -++\rangle)$
(F) $\frac{1}{\sqrt{2}}(-+> + +->)$
(G) $\frac{1}{2}(+++> + -+> + -+> + +->)$
(H) $\frac{1}{2}(+++> + -+> + ---> + -+->)$ |
|---|--|
-

Quantum Field Theory

In this problem we consider the chiral representation, and write a Dirac spinor ψ in terms of two chiral spinors ψ_L and ψ_R as $\psi = [\psi_L, \psi_R]^\top$. The Lagrangian density for the Dirac theory contains a mass term of the form

$$\mathcal{L} = \dots + im\bar{\psi}\psi = \dots + im(\psi_L^\dagger \psi_R + \psi_R^\dagger \psi_L).$$

Statements

1. The above mass term is Lorentz invariant.
 2. $m\psi_L^\dagger \psi_L$ is Lorentz invariant.
 3. $m\psi_R^\dagger \psi_R$ is Lorentz invariant.
- (A) 1. True, 2. True, 3. True (B) 1. True, 2. True, 3. False (C) 1. True, 2. False, 3. True (D) 1. True, 2. False, 3. False
 (E) 1. False, 2. True, 3. True (F) 1. False, 2. False, 3. False (G) 1. False, 2. True, 3. False (H) 1. False, 2. False, 3. True
-

Optics

The Lloyd mirror is a wavefront-splitting interferometer. It consists of a flat glass mirror that reflects a portion of wavefront that comes from a narrow slit. Another portion of the wavefront proceeds directly to the screen. The interference of the two wavefronts form a set of bright and dark fringes that can be measured on the screen.

In our problem, let's assume the mirror is placed at the plane $x = 0$ and illuminated by a spherical wave originating from the slit at location $(x_0, -z_0)$ (where $x_0, z_0 > 0$). Using the paraxial approximation for a 1D spherical wave ($y = 0$),

$$E(x, z) = E_0 \frac{\exp[i(k(z + z_0))]}{i(z + z_0)} \exp\left[ik \frac{(x - x_0)^2}{2(z + z_0)}\right]$$

The source illuminating the slit has a wavelength of 500nm in air. If the slit is positioned at $x_0 = 1\text{mm}$ above the flat mirror, and the screen is placed 1 meter away from the slit, please estimate the spacing of the fringes on the screen.

- | | | | |
|--------------------------|--------------------------|----------------------------|---------------------------|
| (A) 25 mm
(E) 0.25 mm | (B) 500 mm
(F) 250 mm | (C) 0.75 mm
(G) 0.50 mm | (D) 100 mm
(H) 1.00 mm |
|--------------------------|--------------------------|----------------------------|---------------------------|
-

Table 5: Examples of questions included in QuantumBench. From three fields, examples are given for algebraic calculation, conceptual understanding, and numerical calculation.

solving models achieve accuracy comparable to large non-reasoning models even with fewer parameters. Figure 3(c) further confirms the role of reasoning by plotting performance as a function of reasoning strength from minimal to high. Deeper reasoning consistently improves accuracy, with a marked drop at the minimal setting and substantial gains even at the low setting.

This perspective is especially relevant to cost effectiveness. Figure 3(d) shows the relationship between API inference cost and accuracy. Notably, performance gains diminish sharply as cost increases. In other words, even small models, under medium reasoning and low-cost settings, can approach the accuracy of frontier models. These findings indicate that, for AI tools supporting scientific research, adopting small- to medium-scale models with moderate reasoning capabilities as the default configuration can achieve an effective balance between performance and computational cost.

Figure 4 illustrates accuracy by question category for some frontier and mid-tier models from each provider. In Optics, prior or non-reasoning models achieved only limited accuracy, whereas large reasoning models approached 80%. Many Optics questions rely on diagrammatic or spatial information such as lens placement, relative spacing, and propagation direction, which is difficult to process linguistically and is considered one factor underlying this performance gap. Similarly, fields such as String Theory, Quantum Field Theory, and Nuclear Physics demand relatively advanced domain knowledge and reasoning, resulting in a larger variance in accuracy across models.

Figure 4(b) shows accuracy by question type. There were no notable behavioral differences among the models across problem types. GPT-5-high, which achieved the highest overall accuracy, consistently outperformed the other models across all three question types.

Figure 5 shows the relationship between model

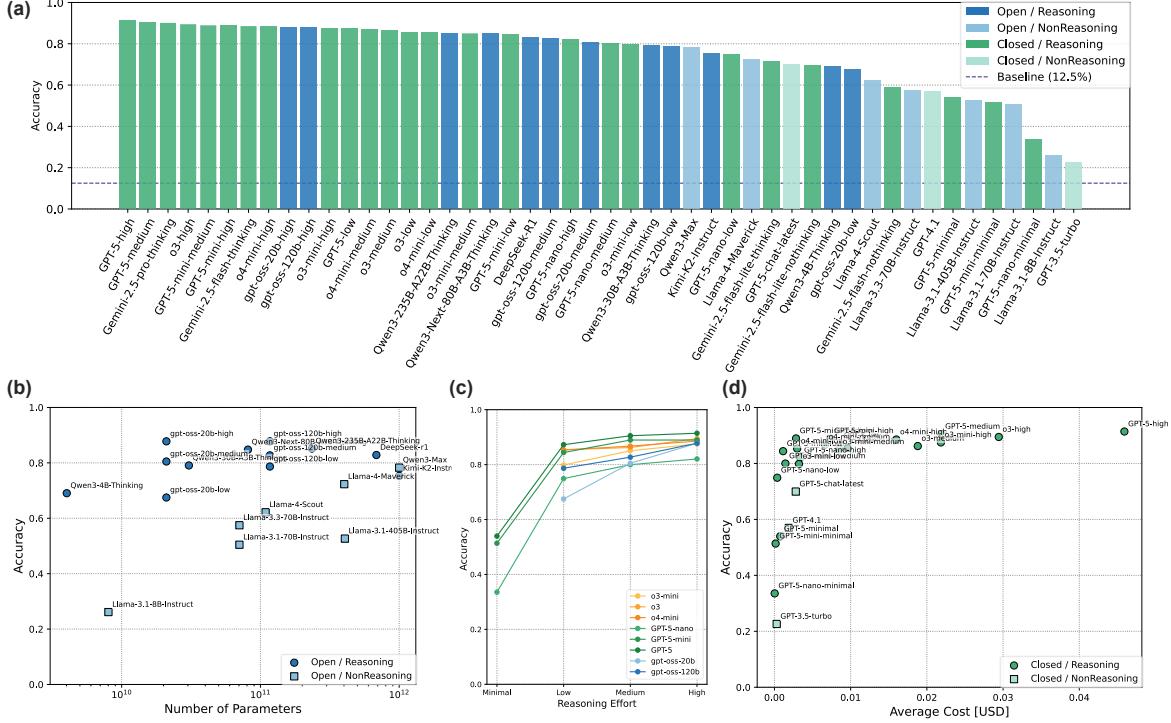


Figure 3: Benchmark results. (a) Accuracy on all 769 problems. Blue indicates open-weight models, and green indicates closed models available only via API. Dark colors denote reasoning models, while light colors denote non-reasoning models. Tags appended to the names of reasoning models indicate the strength of reasoning. (b) Relationship between the number of model parameters and accuracy. Only open-weight models with publicly available parameter counts are shown. Blue circles represent reasoning models, and light-blue squares represent non-reasoning models. (c) Transition of accuracy when varying the reasoning strength for reasoning models. The “minimal” setting is available only for some models. (d) Relationship between average API usage cost per problem and accuracy. Only closed models, which require API usage, are shown. Green circles represent reasoning models, and light-green circles represent non-reasoning models.

accuracy and both difficulty and expertise levels. In both categories, accuracy declined progressively as the level increased. However, the decrease was relatively moderate, and no statistically significant differences in performance were observed between difficulty levels 2 (easy) and 3 (standard) or between expertise levels 1 (high school) and 2 (undergraduate). These findings suggest that errors on problems of medium-level difficulty or expertise are driven by factors other than difficulty or expertise alone. Section 4.3 provides a detailed analysis of these error sources.

4.2. Zero-Shot CoT

Zero-shot CoT (Kojima et al., 2022) is a prompting method that directs the model to perform chain-of-thought (CoT) reasoning without examples, thereby inducing step-by-step inference. We applied zero-shot CoT to ten non-reasoning models and examined the resulting performance improvements.

Figure 6(a) shows the accuracy gains obtained with zero-shot CoT. Although accuracy improved for

many models, the magnitude of improvement was generally limited. Some of high-performing models, such as Qwen3-Max, GPT-5-chat-latest, and GPT-4.1 showed the most pronounced gains, whereas many prior models with low base performance exhibited only minor improvements. This indicates that models lacking sufficient baseline ability cannot achieve substantial improvement through simple prompting-based reasoning techniques. The notable improvement observed in GPT-4.1 is likely due to its ability to process very long contexts (exceeding one million tokens), allowing for extended reasoning steps.

As models are prompted to perform deeper reasoning, the number of generated tokens and associated inference cost increase. Figure 6(b) illustrates this rise in inference cost when zero-shot CoT is applied. GPT-4.1, which achieved the largest accuracy gain, also incurred a significant cost increase due to the generation of long-form reasoning traces. In contrast, GPT-5-chat-latest also showed an increase in cost, while the performance improvement was limited. This observation implies that questions

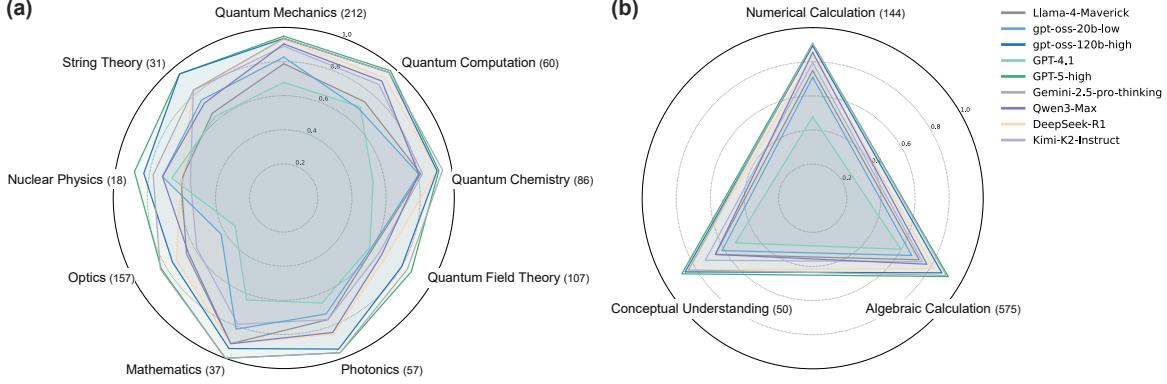


Figure 4: Category-wise accuracy of the LLMs. (a) Accuracy by question domain. The numbers attached to the axis labels indicate the number of questions in each domain. (b) Accuracy by question type.

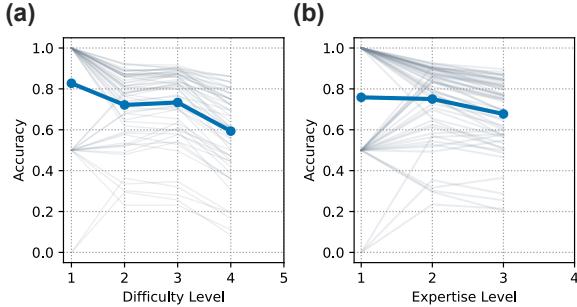


Figure 5: Accuracy of LLMs across (a) difficulty and (b) expertise levels. Each gray line shows the accuracy of an individual model, and the blue line shows the average accuracy across all models.

that remain unsolved by high-performing models under zero-shot settings cannot be resolved simply by extending elementary reasoning procedures. In other words, current models still struggle to construct effective reasoning chains for complex scientific questions. Because many quantum-domain tasks require long step-by-step theoretical analyses, models must be trained to develop robust long-form reasoning steps.

4.3. Error Analysis

Systematic analysis of common or characteristic error patterns in LLMs supports high-accuracy deployment in practical applications. Figure 7 presents a representative case in which the experts rated the question as level 2 (easy), yet the average accuracy across the evaluated LLMs was only about 29.2%. The figure also displays the reasoning process produced by gpt-oss-120b-high. The task asks whether two operators constitute a complete set of commuting observables (CSCO). A correct solution requires verifying a sequence of necessary conditions and then concluding that the operators form a CSCO. The model skipped part of this verification and therefore produced the incorrect

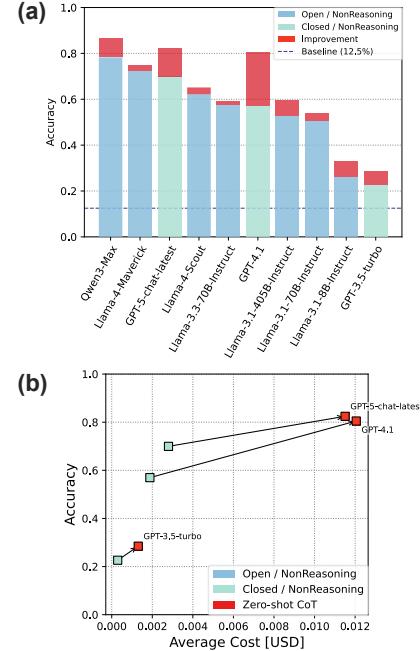


Figure 6: Performance changes with zero-shot CoT. (a) Accuracy of non-reasoning models in the zero-shot setting, and the improvement with zero-shot CoT. Blue indicates open-weight models, and green indicates closed models. The red area represents the improvement margin due to zero-shot CoT. (b) Transition of accuracy and inference cost when zero-shot CoT is applied.

conclusion that they do not.

Failures to perform the necessary reasoning steps in scientific contexts constitute one of the primary sources of error on QuantumBench and have also been documented in the prior work (Pan et al., 2025). Other frequent causes include excessive reliance on common sense at the expense of the stated definitions and assumptions, errors in handling indices and signs, and failure to follow instructions, which often leads the model to report a different target quantity. Systematically mitigat-

Question					
Is $\{L_{xy}, L_z\}$ a complete set of commuting observables? Here L_x and L_y are angular momentum operators corresponding to rotations around the x - and y -axis, and $L_{xy} = L_x^2 + L_y^2$.					
LLM response					
Set $\{L_{xy}, L_z\}$. $L_{xy} = L_x^2 + L_y^2$. Do they commute? Compute $[L_{xy}, L_z] = [L_x^2 + L_y^2, L_z] = [L_x^2, L_z] + [L_y^2, L_z]$. (...) Sum cancels: $i\hbar(\dots) - i\hbar(\dots) = 0$. So they commute. Is $\{L_{xy}, L_z\}$ a complete set of commuting observables? (...) So possibly yes a CSCO for angular momentum. However does L_{xy} have degenerate eigenvalues for different j, m ? (...) ($j = 1, m = 0$) and ($j = 2, m = \pm 2$) give same $L_{xy} = 2\hbar^2$. Therefore $\{L_{xy}, L_z\}$ does not uniquely specify the state; not complete.					

Figure 7: An example of incorrect responses by LLMs. We extract a snippet of the question and the reasoning process. The red text indicates the errors in the reasoning. The LLM claims incompleteness by presenting an example where L_{xy} takes the same value, but since L_z differs, the example is not a valid counterexample.

ing these tendencies is essential for building more accurate and trustworthy AI systems.

4.4. Bias Analysis for LLM-as-a-Judge

We examined whether an LLM can appropriately judge the level of difficulty and expertise. We used GPT-5-chat-latest to assign difficulty and expertise levels to each QuantumBench question and compared these labels with human annotations. The decision criteria embedded in the prompts matched those in Tables 3 and 4.

Figure 8 summarizes the correspondence between LLM and human labels. In the difficulty annotation task, the LLM rated the questions as more difficult than human experts: while humans placed most questions at Level 2 (easy) or Level 3 (standard), the LLM’s labels were roughly uniform across Levels 2–4. A similar trend held in the expertise annotation task: the LLM tended to judge the questions as requiring higher levels of expertise than human experts.

Several factors may account for these discrepancies. First, while the LLM appears to recognize that most problems do not fall into the extreme difficulty levels (Levels 1 and 5), it may have failed to reliably distinguish among the intermediate categories (Levels 2–4). Consequently, the model likely assigned labels within that range uniformly at random. In addition, multiple biases have been noted when using LLMs as judges. For example, a verbosity bias has been observed, in which longer responses tend to be rated more favorably (Zheng et al., 2023; Ye et al., 2024). In the evaluation of mathematical content, judgments often reflect stylistic features rather than substantive correctness (Stephan et al., 2024). Given that many QuantumBench items contain detailed problem descriptions and numerous equations, these characteristics may have ampli-

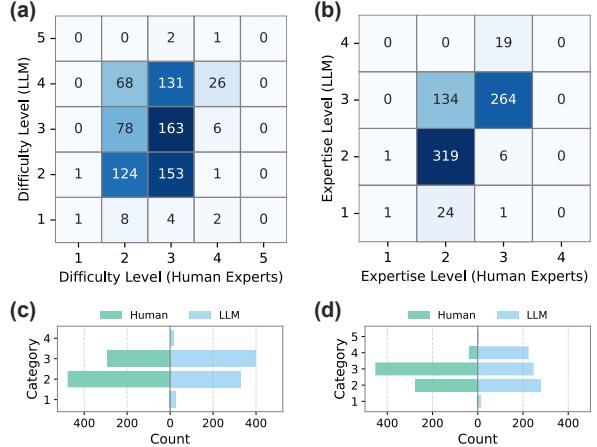


Figure 8: Differences in difficulty and expertise ratings between humans and the LLM. (a, c) Heatmap comparing human and LLM ratings. (b, d) Distribution of human and LLM ratings.

fied such biases, leading the LLM to overestimate the difficulty and degree of expertise required even for fundamentally elementary problems.

5. Conclusion

In this study, we introduced QuantumBench, a benchmark for evaluating LLMs in the quantum domain, constructed from publicly available lecture materials. The dataset comprises 769 undergraduate-level multiple-choice problems across nine areas spanning core and related quantum fields. Using this benchmark, we evaluated existing models, including current frontier models, and analyzed performance by model type, reasoning strength, and computational cost. We found that small to medium models can approach the accuracy of frontier models when prompted with moderate reasoning. We also observed that performance improvements diminish with increasing reasoning strength and clarified that practical performance can be attained even under low-cost settings.

QuantumBench is the first benchmark specialized for LLM evaluation in the quantum domain and supports the advancement of LLM use in quantum science. However, because the dataset is drawn from undergraduate and graduate course materials, it does not fully capture the difficulty, quality, or formats characteristic of cutting-edge research and development. Many real-world research tasks are not multiple choice but instead require goal specification, procedural decomposition, verification, and interpretation. To develop more sophisticated AI scientists, future benchmarks should include more practical tasks such as open-ended descriptive questions, structured task decomposition, and systematic experiment planning.

6. Limitations

Because the dataset was constructed from course materials that are publicly available on the web, the underlying sources and related resources may have been included in the training corpora of LLMs. In most of these sources, however, problems and solutions are distributed in separate files, which makes it difficult for an LLM to memorize exact problem-answer pairs. In addition, we have edited the problem statements and newly created all choices. These processes mitigate training-data contamination and keep the dataset suitable for evaluation.

We further evaluated model performance on a Japanese version of the benchmark and found that results were very similar to those on the English original, indicating that models are not merely recalling memorized question–answer pairs.

Because enlisting domain experts across all sub-fields in the dataset was infeasible, we did not measure human accuracy on the benchmark. Instead, the physics experts assigned categorical ratings for difficulty and expertise level. From the standpoint of evaluating LLM capabilities, establishing a human baseline remains desirable and is deferred to future work.

7. Ethics Statements

7.1. License

All source lecture materials were distributed under the CC BY-NC-SA license, and the dataset created in this study is distributed under the same license. The title of each source lecture, the lecturer’s name, and the lecture URL are explicitly included as metadata within the dataset.

7.2. Human Annotations

The annotation was conducted by three of the authors. Prior to the task, we held a meeting to share the details of the annotation process and provided a comprehensive annotation guideline to standardize the evaluation criteria and working procedures. The annotators understood and agreed that their work would be released as part of the dataset. During the annotation process, we communicated with the annotators as needed to discuss how to handle irregular cases.

8. Bibliographical References

Josh Achiam, Steven Adler, Sandhini Agarwal, Lama Ahmad, Ilge Akkaya, Florencia Leoni Aleman, Diogo Almeida, Janko Altenschmidt, Sam Altman, Shyamal Anadkat, et al.

2023. GPT-4 technical report. *arXiv preprint arXiv:2303.08774*.

Sandhini Agarwal, Lama Ahmad, Jason Ai, Sam Altman, Andy Applebaum, Edwin Arbus, Rahul K Arora, Yu Bai, Bowen Baker, Haiming Bao, et al. 2025. gpt-oss-120b & gpt-oss-20b model card. *arXiv preprint arXiv:2508.10925*.

Samuel R Bowman, Jeeyoon Hyun, Ethan Perez, Edwin Chen, Craig Pettit, Scott Heiner, Kamilé Lukošiūtė, Amanda Askell, Andy Jones, Anna Chen, et al. 2022. Measuring progress on scalable oversight for large language models. *arXiv preprint arXiv:2211.03540*.

Tom Brown, Benjamin Mann, Nick Ryder, Melanie Subbiah, Jared D Kaplan, Prafulla Dhariwal, Arvind Neelakantan, Pranav Shyam, Girish Sastry, Amanda Askell, et al. 2020. Language models are few-shot learners. *Advances in neural information processing systems*, 33:1877–1901.

Shuxiang Cao, Zijian Zhang, Mohammed Alghadeer, Simone D Fasciati, Michele Piscitelli, Mustafa Bakr, Peter Leek, and Alán Aspuru-Guzik. 2025. Automating quantum computing laboratory experiments with an agent-based AI framework. *Patterns*.

Delft University of Technology. TU Delft OpenCourseWare. <https://ocw.tudelft.nl/>.

Abhimanyu Dubey, Abhinav Jauhri, Abhinav Pandey, Abhishek Kadian, Ahmad Al-Dahle, Aiesha Letman, Akhil Mathur, Alan Schelten, Amy Yang, Angela Fan, et al. 2024. The Llama 3 herd of models. *arXiv e-prints*, pages arXiv-2407.

Nicolas Dupuis, Luca Buratti, Sanjay Vishwakarma, Aitana Viudes Forrat, David Kremer, Ismael Faro, Ruchir Puri, and Juan Cruz-Benito. 2024. Qiskit code assistant: Training LLMs for generating quantum computing code. In *2024 IEEE LLM Aided Design Workshop (LAD)*, pages 1–4. IEEE.

Steffen Eger, Yong Cao, Jennifer D’Souza, Andreas Geiger, Christian Greisinger, Stephanie Gross, Yufang Hou, Brigitte Krenn, Anne Lauscher, Yizhi Li, et al. 2025. Transforming science with large language models: A survey on AI-assisted scientific discovery, experimentation, content generation, and evaluation. *arXiv preprint arXiv:2502.05151*.

Gemini Team. 2023. Gemini: a family of highly capable multimodal models. *arXiv preprint arXiv:2312.11805*.

- Daya Guo, Dejian Yang, Haowei Zhang, Junxiao Song, Ruoyu Zhang, Runxin Xu, Qihao Zhu, Shirong Ma, Peiyi Wang, Xiao Bi, et al. 2025. DeepSeek-R1: Incentivizing reasoning capability in LLMs via reinforcement learning. *arXiv preprint arXiv:2501.12948*.
- Ali Javadi-Abhari, Matthew Treinish, Kevin Krsulich, Christopher J. Wood, Jake Lishman, Julien Gacon, Simon Martiel, Paul D. Nation, Lev S. Bishop, Andrew W. Cross, Blake R. Johnson, and Jay M. Gambetta. 2024. Quantum computing with Qiskit. *arXiv preprint arXiv:2405.08810*.
- Jared Kaplan, Sam McCandlish, Tom Henighan, Tom B Brown, Benjamin Chess, Rewon Child, Scott Gray, Alec Radford, Jeffrey Wu, and Dario Amodei. 2020. Scaling laws for neural language models. *arXiv preprint arXiv:2001.08361*.
- Kimi Team. 2025. Kimi K2: Open agentic intelligence. *arXiv preprint arXiv:2507.20534*.
- Takeshi Kojima, Shixiang Shane Gu, Machel Reid, Yutaka Matsuo, and Yusuke Iwasawa. 2022. Large language models are zero-shot reasoners. *Advances in neural information processing systems*, 35:22199–22213.
- LibreTexts. LibreTexts. <https://libretexts.org/>.
- Chris Lu, Cong Lu, Robert Tjarko Lange, Jakob Foerster, Jeff Clune, and David Ha. 2024. The ai scientist: Towards fully automated open-ended scientific discovery. *arXiv preprint arXiv:2408.06292*.
- Laurens van der Maaten and Geoffrey Hinton. 2008. Visualizing data using t-sne. *Journal of machine learning research*, 9(Nov):2579–2605.
- Massachusetts Institute of Technology. MIT OpenCourseWare. <https://ocw.mit.edu/>.
- Haining Pan, Nayantara Mudur, William Taranto, Maria Tikhonovskaya, Subhashini Venugopalan, Yasaman Bahri, Michael P Brenner, and Eun-Ah Kim. 2025. Quantum many-body physics calculations with large language models. *Communications Physics*, 8(1):49.
- Samuel Schmidgall, Yusheng Su, Ze Wang, Ximeng Sun, Jialian Wu, Xiaodong Yu, Jiang Liu, Michael Moor, Zicheng Liu, and Emad Barssoum. 2025. Agent laboratory: Using LLM agents as research assistants. *arXiv preprint arXiv:2501.04227*.
- Andreas Stephan, Dawei Zhu, Matthias Aßmacher, Xiaoyu Shen, and Benjamin Roth. 2024. From calculation to adjudication: Examining LLM judges on mathematical reasoning tasks. *arXiv preprint arXiv:2409.04168*.
- Hugo Touvron, Thibaut Lavril, Gautier Izacard, Xavier Martinet, Marie-Anne Lachaux, Timothée Lacroix, Baptiste Rozière, Naman Goyal, Eric Hambro, Faisal Azhar, et al. 2023. Llama: Open and efficient foundation language models. *arXiv preprint arXiv:2302.13971*.
- Yutaro Yamada, Robert Tjarko Lange, Cong Lu, Shengran Hu, Chris Lu, Jakob Foerster, Jeff Clune, and David Ha. 2025. The ai scientist-v2: Workshop-level automated scientific discovery via agentic tree search. *arXiv preprint arXiv:2504.08066*.
- An Yang, Anfeng Li, Baosong Yang, Beichen Zhang, Binyuan Hui, Bo Zheng, Bowen Yu, Chang Gao, Chengan Huang, Chenxu Lv, et al. 2025. Qwen3 technical report. *arXiv preprint arXiv:2505.09388*.
- Jiayi Ye, Yanbo Wang, Yue Huang, Dongping Chen, Qihui Zhang, Nuno Moniz, Tian Gao, Werner Geyer, Chao Huang, Pin-Yu Chen, et al. 2024. Justice or prejudice? quantifying biases in llm-as-a-judge. *arXiv preprint arXiv:2410.02736*.
- Lianmin Zheng, Wei-Lin Chiang, Ying Sheng, Siyuan Zhuang, Zhanghao Wu, Yonghao Zhuang, Zi Lin, Zuhuan Li, Dacheng Li, Eric Xing, et al. 2023. Judging LLM-as-a-judge with MT-Bench and Chatbot Arena. *Advances in neural information processing systems*, 36:46595–46623.
- Yunheng Zou, Austin H Cheng, Abdulrahman Al-dossary, Jiaru Bai, Shi Xuan Leong, Jorge Arturo Campos-Gonzalez-Angulo, Changhyeok Choi, Cher Tian Ser, Gary Tom, Andrew Wang, et al. 2025. El agente: An autonomous agent for quantum chemistry. *Matter*, 8(7).

9. Language Resource References

- Hendrycks, Dan and Burns, Collin and Basart, Steven and Zou, Andy and Mazeika, Mantas and Song, Dawn and Steinhardt, Jacob. 2020. *Measuring massive multitask language understanding*.
- Hendrycks, Dan and Burns, Collin and Kadavath, Saurav and Arora, Akul and Basart, Steven and Tang, Eric and Song, Dawn and Steinhardt, Jacob. 2021. *Measuring mathematical problem solving with the MATH dataset*.

Jin, Qiao and Dhingra, Bhuvan and Liu, Zhengping and Cohen, William W and Lu, Xinghua. 2019. *PubMedQA: A dataset for biomedical research question answering*.

Shlomo Kashani. 2024. QuantumLLMInstruct: A 500k LLM instruction-tuning dataset with problem-solution pairs for quantum computing. *arXiv preprint arXiv:2412.20956*.

Mikuriya, Taku and Ishigaki, Tatsuya and Minami, Shunya and Kadowaki, Tadashi and Suzuki, Yohichi and Naito, Shun and Takada, Shunya and Kato, Takumi and Baseda, Tamotsu and Yamada and, Reo and Takamura, Hiroya. 2025. *QCoder Benchmark: Bridging language generation and quantum hardware through simulator-based feedback*.

Phan, Long and Gatti, Alice and Han, Ziwen and Li, Nathaniel and Hu, Josephina and Zhang, Hugh and Zhang, Chen Bo Calvin and Shaaban, Mohamed and Ling, John and Shi, Sean and others. 2025. *Humanity's last exam*.

Rein, David and Hou, Betty Li and Stickland, Asa Cooper and Petty, Jackson and Pang, Richard Yuanzhe and Dirani, Julien and Michael, Julian and Bowman, Samuel R. 2024. *GPQA: A graduate-level google-proof Q&A benchmark*.

Vishwakarma, Sanjay and Harkins, Francis and Golecha, Siddharth and Bajpe, Vishal Sharathchandra and Dupuis, Nicolas and Buratti, Luca and Kremer, David and Faro, Ismael and Puri, Ruchir and Cruz-Benito, Juan. 2024. *Qiskit HumanEval: An evaluation benchmark for quantum code generative models*. IEEE.

Wang, Yubo and Ma, Xueguang and Zhang, Ge and Ni, Yuansheng and Chandra, Abhranil and Guo, Shiguang and Ren, Weiming and Arulraj, Aaran and He, Xuan and Jiang, Ziyan and others. 2024. *MMLU-Pro: A more robust and challenging multi-task language understanding benchmark*.

Zhu, Minhui and Tian, Minyang and Yang, Xiaocheng and Zhou, Tianci and Zhu, Penghao and Chertkov, Eli and Liu, Shengyan and Du, Yufeng and Yuan, Lifan and Ji, Ziming and others. 2025. *Probing the Critical Point (CritPt) of AI Reasoning: a Frontier Physics Research Benchmark*.