MATTHEW DUSCHENES

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SUMMARY

A PhD candidate (graduating Spring, 2026) who loves spreading a joy for learning and empathy at the University of Waterloo, with the late Dr. Raymond Laflamme, Dr. Juan Carrasquilla, and Dr. Roger Melko. An NSERC PGS-D scholarship recipient, a graduate of the University of Michigan Applied Physics and Scientific Computing Master's programs, a graduate of the Perimeter Scholars International Master's program, and an Engineering Physics graduate of Queen's University. Research interests in theoretical and computational approaches to assess the abilities of quantum technologies. Experienced in developing and delivering materials in physics, machine-learning, and statistics disciplines. An ambitious and passionate learner and teacher who collaborates to develop new techniques efficiently within a challenging environment.

SKILLS

Communication and Outreach

- Effective project leader (international 3 year project with 4+ senior and junior members).
- Empathetic mentor (5+ undergraduate and master's student mentees and projects).
- Experienced course content developer and guest lecturer (5+ courses, 8+ guest lectures).
- Outreach contributor (5+ years of public and academic outreach within the scientific community).

Numerical Methods and Software

- Tensor network methods; open quantum system simulation; constrained optimization; graph-theoretic approaches; Bayesian and Monte Carlo methods; generative modelling.
- Python (JAX, Sympy), C++ (Eigen), Latex, Linux/Bash scripting languages.

EXPERIENCE

Graduate Research Assistant **Fall, 2021 - Present**

Department of Physics, University of Waterloo

- Developed theoretical and numerical approaches to investigate dynamics of quantum systems.
- Resolved open questions regarding the impact of noise on the current abilities of quantum computing technologies, with respect to their optimization, statistics, and simulation.

Research Intern **Summer, 2023 - Present**

Los Alamos National Laboratory

- Selected as one of 20 from 600 graduate students for the Quantum Computing Summer School.
- Developed analytical tools to resolve open questions regarding statistics in quantum systems.
- Multi-year project lead of team of 4 faculty from Los Alamos (New Mexico), EPFL (Lausanne), and Institute for Quantum Computing (Waterloo), with several deliverables and presentations.

Guest Lecturer - Dimensional Reduction and Generative Modelling **Fall, 2025**

University of Waterloo and Perimeter Institute

- Machine Learning - PHYS 449: Lecture on dimensional reduction techniques (PCA and t-SNE), derivations of their physically motivated equations, and demonstrations with code examples.
- Statistical Physics - PSI 602: Lecture on generative modelling and its connections to statistical physics, and derivations of intuitive equations used in Restricted Boltzmann Machines.

Teaching Assistant - Quantum Computing Implementations - PHYS 468 **Fall, 2024**
University of Waterloo

- Assisted with lectures, office hours, and grading for 30 students, with Dr. Raymond Laflamme.
- Developed course lecture notes; edited course textbook (Building Quantum Computers, 2024).

Teaching Assistant - Perimeter Scholar's International Start Program **Summer, 2024**
Perimeter Institute

- Delivered tutorials and mentored students on analytical and numerical approaches in physics.

Teaching Assistant - Electricity and Magnetism - PHYS 242 **Winter, 2023-2024**
University of Waterloo

- Assisted with lectures, office hours, and grading for 50 students, with Dr. Raymond Laflamme.
- Developed assignment questions; delivered guest lectures on energy of electromagnetic fields.

Lecturer - International Summer School for Young Physicists **Summer, 2022-2023**
Perimeter Institute

- Developed and delivered 1-week course on undergraduate statistical and computational physics.

Teaching Assistant - Machine Learning Certificate Program **Winter, 2022**
Vector Institute

- Developed and delivered course content on introduction to linear algebra and statistics topics.
- Lead office hour sessions and graded summative assessments for 40 students.

EDUCATION

Physics PhD Program **Fall, 2021 - Summer, 2026**
University of Waterloo, Institute for Quantum Computing, Perimeter Institute

- *Publications, Conferences, and Symposia:*
  - Duschenes, M., Garcia-Martin, D., Holmes, Z. & Cerezo, M. Moments of quantum channel ensembles. *(In Preparation for arXiv), Report: LA-UR-24-20854* (2025)
  - Duschenes, M., Martin, D., Larocca, M., Holmes, Z. & Cerezo, M. "Connecting channel expressiveness to gradient magnitudes and noise induced barren plateaus" (2024). APS March Meeting, Session T51: Quantum Machine Learning Training and Beyond
  - Duschenes, M., Carrasquilla, J. & Laflamme, R. Characterization of overparametrization in the simulation of realistic quantum systems. *Physical Review A* **109**, 062607 (2024)

Applied Physics and Scientific Computing Master's Degree **Fall, 2018 - Summer, 2021**
University of Michigan, Michigan Institute for Computational Discovery & Engineering

- Research on graph-theoretic approaches for high dimensional systems, with Dr. Krishna Garikipati.
- *Publications:*
  - Duschenes, M., Srivastava, S. & Garikipati, K. Numerical analysis of non-local calculus on finite weighted graphs. *Comput. Methods Appl. Mech. Eng.* **402**, 115513 (2022)

Perimeter Scholars International Master's Degree **Summer, 2017 - Spring, 2018**
Perimeter Institute

Engineering Physics, Electrical Specialization Bachelor's Degree **Fall, 2013 - Spring, 2017**
Queen's University

ACTIVITIES AND INTERESTS

Fundamentals of University Teaching Certificate Program **2025**
University of Waterloo

- 6 workshops (Effective Lesson Plans, Classroom Delivery Skills, STEM Tutorials, Giving and Receiving Feedback, Effective Question Strategies, Reflecting on Diversity).
- 3 teaching sessions, where lesson plans are developed and delivered as interactive lessons using the BOPPS and SMART models, in front of a panel.
- 30 hour course on preparation of teaching materials within academia.

Academic and Scientific Communication Programs **2021 - Present**
Perimeter Institute

- Contributor to scientific outreach PSI-START and Einstein+ programs; tour guide for public open houses, delivered guest lectures to public and academic Quetzal and Girls-In-Quantum programs; developed and presented 4 talks on quantum computing for high school students.
- Chair of graduate student seminar series; invited speakers and organized workshops.
- Co-coordinator of high school scientific outreach program; mentored students with their presentations.
- Member of the gender equity in physics working group; mentor of 4 Perimeter master's students; mentor of undergraduate researcher; student representative on scientific communication committees.

Journal and Conference Reviewer **2023 - Present**
Various Organizations

- Reviewer for npj, Phys. Rev, IOP journals, and QCTIP, TQC conferences.

Varsity Cross Country and Track and Field Teams **2013 - 2017**
Queen's University

- Competed year-round across North America in long distance running, and coordinated workouts.

AWARDS

NSERC PGS-D Graduate Scholarship **2023 - 2026**
Natural Sciences and Engineering Research Council of Canada ($100,000)

President's Award, Marie Curie Award, Physics Department Fellowship **2023 - 2026**
University of Waterloo ($24,000)

Vector Research Grant **2022 - 2025**
Vector Institute ($24,000)

Applied Physics Graduate Fellowship **2018 - 2020**
Applied Physics Program, University of Michigan ($50,000)

Perimeter Scholar's International Scholarship **2017 - 2018**
Perimeter Institute and University of Waterloo ($45,000)

Principal's Scholarship, W.W. King Scholarship **2013 - 2014**
Faculty of Applied Science, Queen's University ($24,000)

REFERENCES

References available upon request.

Publications

[1] Duschenes, M. *Distinguishing phases and detecting local and non-local order using t-SNE and Monte Carlo methods.* Master's thesis, Perimeter Scholar's International Essays, Perimeter Institute, Waterloo, Ontario (2018).

[2] Kochunas, B., Garikipati, K., Duschenes, M. & Folk, T. The graph theoretic approach for nodal cross section parameterization (2020). arXiv:2010.09683 [physics.comp-ph].

[3] Duschenes, M. & Garikipati, K. Reduced order models from computed states of physical systems using non-local calculus on finite weighted graphs (2021). arXiv:2105.01740 [math.NA].

[4] Price, D., Folk, T., Duschenes, M., Garikipati, K. & Kochunas, B. Methodology for Sensitivity Analysis of Homogenized Cross-Sections to Instantaneous and Historical Lattice Conditions with Application to AP1000® PWR Lattice. *Energies* **14**, 3378 (2021).

[5] Zhang, X., Teichert, G. H., Wang, Z., Duschenes, M., Srivastava, S., Sunderarajan, A., Livingston, E. & Garikipati, K. mechanoChemML: A software library for machine learning in computational materials physics. *Computational Materials Science* **8**, 111493 (2022).

[6] Duschenes, M., Srivastava, S. & Garikipati, K. Numerical analysis of non-local calculus on finite weighted graphs. *Comput. Methods Appl. Mech. Eng.* **402**, 115513 (2022).

[7] Duschenes, M., Carrasquilla, J. & Laflamme, R. Characterization of overparametrization in the simulation of realistic quantum systems. *Physical Review A* **109**, 062607 (2024).

[8] Duschenes, M. simulation: Jax based simulator for quantum systems (2022). https://github.com/mduschenes/simulation.

[9] Duschenes, M., Garcia-Martin, D., Holmes, Z. & Cerezo, M. Moments of quantum channel ensembles. *(In Preparation for arXiv), Report: LA-UR-24-20854* (2025).

[10] Duschenes, M., Melko, R., Carrasquilla, J. & Laflamme, R. Simulation of Noisy Quantum Systems with POVM Probabilities. *(In Preparation for arXiv)* (2025).

Seminars

[1] Duschenes, M. “Graph theoretic approaches for physical systems”. In *UM Phys. Grad. Student Symp.* (2020).

[2] Duschenes, M. “Reduced order modelling on finite weighted graphs”. In *MICDE Student Semin.* (2021).

[3] Duschenes, M. “Reduced order models using non-local calculus on unstructured weighted graphs”. In *US Natl. Congr. Comput. Mech.* (2021).

[4] Duschenes, M. “Learning and Overparameterization of Constrained Variational Quantum Circuits”. In *IAIFI Summer School and Workshop* (2022).

[5] Duschenes, M. “Overparameterization of Realistic Quantum Circuits”. In *Perimeter Institute Quantum Matter Workshop* (2022).

[6] Duschenes, M. “Overparameterization of Realistic Quantum Systems”. In *Perimeter Graduate Student Seminar Series* (2022). PIRSA:22110060 see, `https://pirsa.org`.

[7] Duschenes, M. “Overparameterization of Realistic Quantum Systems”. In *Quantum Days Conference* (2023).

[8] Duschenes, M. “Overparameterization of Realistic Quantum Systems”. In *Canadian Quantum Graduate Conference* (2023).

[9] Duschenes, M., J., C. & R., L. “Overparameterization of Realistic Quantum Systems” (2023). APS March Meeting, Session Y70: Quantum System Learning.

[10] Duschenes, M. “Overparameterization of Realistic Quantum Systems”. In *IQC Graduate Quantum Conference* (2023).

[11] Duschenes, M. “Noisy Overparameterization of Quantum Systems”. In *Vector Institute Quantum + Machine Learning Workshop* (2023).

[12] Duschenes, M. “Overparameterization of Realistic Quantum Systems”. In *PI/MILA Quantum/AI Workshop* (2023).

[13] Duschenes, M., Martin, D., Larocca, M., Holmes, Z. & Cerezo, M. “Connecting channel expressiveness to gradient magnitudes and noise induced barren plateaus” (2024). APS March Meeting, Session T51: Quantum Machine Learning Training and Beyond.

[14] Duschenes, M. “Expressivity measures of quantum channels and their operational meaning”. In *Perimeter Graduate Student Seminar Series* (2024). PIRSA:24040122 see, `https://pirsa.org`.

[15] Duschenes, M. Overparameterization and expressivity of realistic quantum systems (2024). Invited Talks - IBM Zurich (Christa Zoufal), Freie Universität Berlin (Jens Eisert Group), EPFL (Zoe Holmes Group).

[16] Duschenes, M. “Channel Expressivity Measures”. In *IQC Graduate Student Conference* (2024).

[17] Duschenes, M. “Channel Expressivity Measures”. In *Perimeter Graduate Student Conference* (2024). PIRSA:24090201 see, `https://pirsa.org`.

[18] Duschenes, M. “Expressivity measures of quantum channels and their operational meaning”. In *CQIQC Conference X* (2024).

[19] Duschenes, M. “Moments of Quantum Channels”. In *Benasque Quantum Information* (2025).

[20] Duschenes, M. Moments of quantum channels (2025). Invited Talk - IFCO Barcelona (Antonio Acin Group).

[21] Duschenes, M. "Simulation of Noisy Quantum Systems with POVM-MPS". In *IQC Grad Student Conference* (2025).

[22] Duschenes, M. "Moments of Quantum Channels". In *Quantum Across Canada Conference* (2025).

TEACHING DOSSIER - MATTHEW DUSCHENES

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A PhD candidate at the University of Waterloo, seeking teaching opportunities at the post-secondary level. Experienced in developing course content, guest lecturing, and academic outreach, in physics, machine-learning, and statistics disciplines. Research interests in theoretical and computational approaches to studying quantum information, and the current abilities of quantum technologies. A driven, ambitious, and passionate learner and teacher, who loves spreading a joy for understanding, empathy, and perseverance.

Statement of Teaching Philosophy **2**

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STATEMENT OF TEACHING PHILOSOPHY

As an academic, given the incredible privilege and joy to be able to learn, to teach and to be curious, I seek to instil such feelings in others. Offering opportunities to make connections to previously learned concepts, to persevere to learn concepts at hand, and to get a glimpse into future concepts to be understood, are central aspects of my objectives as an educator. Learning also takes an incredible amount of dedication, and a recognition that skills must be learned incrementally over time. Such patience is a skill in itself, to be honed and encouraged by teachers. Concurrently, teaching must be approached with humility and empathy. There must be a careful balance between what students aim to get out of their education, versus what teachers aim to convey, and adjustments must be continuously made. Underlying these objectives, I believe that any teacher's role, at any level, is to provide others with fundamental and well motivated tools, and the confidence to think critically and arrive at insights about particular and general topics.

Throughout my own academic journey, I have become acutely aware of challenges that students face, particularly in physical sciences. First, physical and mathematical subjects can be incredibly intimidating, technical, and abstract. Second, students may lack confidence in their abilities, or feel unmotivated to learn and to persevere. Third, students may feel isolated, or dismissed by their seniors in the academic hierarchy. Finally, students may feel the both real and presumed pressures of the current intense workload, as well as credentialism, and employment prospects. I aim to directly acknowledge these challenges with my students, and to address these challenges throughout my lecturing and assessment.

When explicitly teaching, I strive for my lessons to feel like discussions between peers. We are all motivated, for various reasons to improve our understanding of a topic at hand. Structuring of lesson plans to include individual and group discussions, encourages camaraderie, and ensures a natural discourse and feedback mechanism. It is particularly important for there to be opportunities for feedback from students, before lessons to solidify previous concepts, during lessons to emphasize new concepts, and after lessons to prepare for future concepts. Students should also be offered several methods of communication, such as via anonymous polls, asynchronous forums, and personal sessions. By explicitly highlighting what students have already learned into a lesson, previous and current concepts may be connected and solidified. New concepts should also be released gradually, through carefully scheduled periods of demonstration, shared practice, and independent application. Finally, while striving for equity and relaxed environments, students must be kept focused, and respectful of the objectives that everyone is trying to accomplish.

In particular for physical sciences, building up physical intuition is equally as important as improving mathematical skills necessary to complete calculations. Examples in my lectures are ideally the simplest cases of problems, and encourage students to take a step back, and think about what answer appears to be the most intuitive. With this destination in mind, students may proceed to reach an answer more formally with mathematics. Such approaches also allow students to build up problem solving strategies, where at each step in the process, they are able to check whether they are on the right track. Students should slowly learn not to be overwhelmed or daunted, but confident to make slow and steady progress, with the clear objective of long-term retention of transferable skills throughout their journey.

Regarding assessment, I ask students to solve relevant, but distinct problems from those seen in class. Students should be challenged to see connections between topics, while also not feeling like they are doing busy-work, but are improving upon various skills. Students should be able to transparently see their own progress, and to see where such assessments and lessons fit into their overall education. I also prefer personalized feedback, in particular concerning students' approaches to questions, rather than narrowly assessing the correctness of their final solutions with solely numerical grading. Such feedback further promotes discussion, encourages students to try many approaches to solving problems, and ensures students are learning about the process and intuition of physical sciences, not just about reaching a result.

Teaching and learning should be a motivated and motivating long term process. I look forward to contributing to the learning environment being more exciting, equitable, and encouraging.

CURRENT AND FUTURE CONTRIBUTIONS TO TEACHING

My motivations for teaching and abilities to convey complex concepts have improved throughout my various teaching and scientific communication experiences.

At the University of Waterloo, I have been a Teaching Assistant, teaching undergraduate courses of 30-40 students for Dr. Raymond Laflamme, in Electricity and Magnetism (PHYS 242 - 2023,2024), and Implementations of Quantum Information Processing (PHYS 468 - 2024). I have also guest lectured for Machine Learning in Physics (PHYS 449 - 2025), and Statistical Physics (PSI 602 - 2025). As a teaching assistant, I gave tutorials on summaries of course content, aided students individually and within groups during office hours, graded assignments, exams and final projects, developed exam and assignment questions, and delivered guest lectures. The PHYS 468 course was based on a recent textbook written by Dr. Laflamme (Building Quantum Computers, 2024), and I edited its chapters, and typed its corresponding lectures notes. As a guest lecturer, I developed and delivered lectures on dimensional reduction and generative modelling techniques and their connections to statistical physics, derived physically motivated equations for their implementations, and demonstrated examples of code and numerical results.

At the Vector Institute, I have been a Teaching Assistant for 40 students for the Machine Learning Certificate Program (2022). Here, I delivered undergraduate level tutorial content on linear algebra, numerical methods, and machine learning topics, aided students during office hours, and assessed final projects. At the Perimeter Institute, I have been an instructor for the International Summer School for Young Physicists (ISSYP - 2022), where I developed and delivered a one week course for 5-10 students on statistical physics at an undergraduate level, including an introduction to statistics, mathematical models for phases of matter, and specific analytical and numerical techniques. Such teaching also involved mentoring 5 participants on academic career paths. Finally, while at the Perimeter Institute, I have also contributed to building a sense of community by participating in each of their outreach and academic programming initiatives, including mentoring master's students, assisting with the PSI-START lectures and Einstein+ teaching programs, volunteering as tour guides for public events, guest lecturing for affiliated Quetzal and Girls-In-Quantum programs, and co-coordinating their local high school outreach series.

Throughout each experience, I have received outstanding feedback concerning my understanding of course content, my ability to explain abstract concepts clearly, my balanced approaches during tutorials, and my passion and ability to engage with everyone involved. I have also been cautioned to occasionally slow down my delivery, or provide additional examples. There have also been several instances where students came from a wide range of backgrounds and did not understand prerequisite material, particularly mathematical concepts. It was necessary, but very beneficial, to adapt and poll the class on their current abilities, revise more appropriate assignment questions, book individual tutorials with students to catch them up on specific concepts, and track their individual progress from their unique starting points. I am further committed to improve my teaching abilities and have completed the University of Waterloo Fundamentals of University Teaching Certificate Program (2025), as well as professional development workshops at various institutions (2017-2025). Many physics topics are difficult to address, and I continuously strive to think of more succinct ways of conveying important concepts and messages.

Getting to share in the learning process has involved successful conveying of concepts, has developed camaraderie within my classes, and has revealed many challenges that teachers and students face throughout education. In addition to fostering a more empathetic academic culture, I am particularly excited about teaching statistics, numerical linear algebra, and quantum information, where mathematics, compute science, numerics, and physics principles all converge. Finally, I would be interested in developing curricula that incorporate the expertise of as many teachers as possible. Making courses widely supported by multiple departments within institutions will further directly increase access to highly relevant material, and will ensure students obtain precisely their desired education. Concurrently, the most appropriate teachers and courses may be paired. I look forward to contributing to producing well rounded, lifelong learners.

TEACHING EXPERIENCES AND EVALUATIONS

Guest Lecturer - Dimensional Reduction and Generative Modelling **Fall, 2025**
University of Waterloo and Perimeter Institute

- Machine Learning - PHYS 449: Lecture on dimensional reduction techniques (PCA and t-SNE), derivations of their physically motivated equations, and demonstrations with code examples.
- Statistical Physics - PSI 602: Lecture on generative modelling and its connections to statistical physics, and derivations of intuitive equations used in Restricted Boltzmann Machines.

Teaching Assistant - Quantum Computing Implementations - PHYS 468 **Fall, 2024**
University of Waterloo

- Assisted with lectures, office hours, and grading for 30 students, with Dr. Raymond Laflamme.
- Developed course lecture notes; edited course textbook (Building Quantum Computers, 2024).
- Professor Feedback (Dr. Raymond Laflamme):
  - Delivering Content and Background Knowledge: *Exceeded Expectations*
  - Engagement with Students: *Exceeded Expectations*
  - Office Hours and Online Discussions: *Exceeded Expectations*
  - Marking: *Exceeded Expectations*
  - Comments: Matthew has been a totally outstanding TA. He has been very dedicated. The students were lucky to have him as one of the TA's. You cannot ask for a better TA.

Teaching Assistant - Electricity and Magnetism - PHYS 242 **Winter, 2023,2024**
University of Waterloo

- Assisted with lectures, office hours, and grading for 50 students, with Dr. Raymond Laflamme.
- Developed exam and assignment questions; delivered guest lectures.
- Professor Feedback (Dr. Raymond Laflamme):
  - Delivering Content and Background Knowledge: *Exceeded Expectations*
  - Engagement with Students: *Exceeded Expectations*
  - Office Hours and Online Discussions: *Exceeded Expectations*
  - Marking: *Exceeded Expectations*
  - Comments: Matt Duschenes has been an outstanding TA. It was a real pleasure to have him as a TA. He was well prepared, responsive, and understood the material really well. I would have him again any time.

Lecturer - International Summer School for Young Physicists **Summer, 2022**
Perimeter Institute

- Developed and delivered 1-week course on undergraduate statistical and computational physics.
- Mentored 5 high school students on career paths within physics and academia.

Teaching Assistant - Machine Learning Certificate Program **Winter, 2022**
Vector Institute

- Developed and delivered course content on introduction to linear algebra and statistics topics.
- Lead office hour sessions and graded summative assessments for 40 students.

- Student Feedback (Anonymous Survey of Participants):
  - Teaching Strengths: "Matt is great in teaching and explaining mathematical subjects." ; "Matt is also very patient with the students." ; "Matt did an exceptional job at taking high level concepts and really breaking down the theory to understand the math tied in with the applications." ; "Matt is very knowledgeable and was really good in terms of explaining the topics and making the sure students understood the concepts well." ; "[Matt] had a lot of patience for all questions asked and always gave his all in the answers. It is very clear that this is a subject matter he is not only passionate in, but also very knowledgeable in."
  - Teaching Weaknesses: "Matt could have used more examples to explain his point [...] Matt could have explained some concepts a little more clearly with more examples." ; "Matt could improve his confidence and sort of downplayed his knowledge."
  - Tutorial Strengths: "Matt gave very clear and concise tutorials which I enjoyed. It was very helpful [tutorials also] included some coding exercises to see how the math was being applied."
  - Tutorial Weaknesses: "I would recommend Matt slow down a bit."

Figure 1: Student Evaluations: Machine Learning Certificate Program (Vector Institute, 2022)

PROFESSIONAL DEVELOPMENT

Fundamentals of University Teaching Certificate Program **2025**
University of Waterloo

- Completion of 6 workshops (Effective Lesson Plans, Classroom Delivery Skills, STEM Tutorials, Giving and Receiving Feedback, Effective Question Strategies, Reflecting on Diversity).
- Completion of 3 teaching sessions, where lesson plans are developed and delivered as interactive lessons using the BOPPS and SMART models, in front of a panel.
- Completion of 30 hour course on preparation of teaching materials within academia.

Perimeter Graduate Scientific Communication Program **2021-Present**
Perimeter Institute

- Monthly workshops on best practices for oral and written scientific communication and academic outreach, both for general public and targeted audiences.
- Instructor for ISSYP, PSI-Start programs within Perimeter, and guest lecturer for Girls-In-Quantum and Quetzal programs external to Perimeter.
- Chair of graduate student seminar series; invited speakers and organized workshops.
- Co-coordinator of high school scientific outreach program; mentored students with their presentations.
- Development of outreach lectures on career paths in academia and introductions to quantum computing for high school students (delivered at Grand River Collegiate Institute, 2025).

Michigan Graduate RELATE Communications Workshop **2020**
University of Michigan

- Weekly lectures on scientific oral communication, and final teaching video deliverable.

Perimeter Scholar's International Scientific Writing Program **2018**
Perimeter Institute

- Weekly lectures on scientific written communication, and final academic paper deliverable.

COURSE MATERIALS

Tutorial Notes - PHYS 242 (Pg. 8 - 11) **Winter, 2024**
University of Waterloo

Example tutorial notes on electricity and magnetism for PHYS 242 (Tutorial 2 - 2024).

Assignment Problems - PHYS 242 (Pg. 12 - 15) **Winter, 2024**
University of Waterloo

Example assignment problems on electricity and magnetism for PHYS 242 (Assignments - 2024).

Lecture Notes - ISSYP (Pg. 16 - 26) **Summer, 2022**
Perimeter Institute

Example lecture notes on statistical physics for the International Summer School for Young Physicists program (Lecture 2 - 2022).

1 Coordinate Transformations

1.1 Curvilinear Coordinates

We will investigate general coordinate basis transformations

$$(x, y, z, \dots) \to (x', y', z', \dots) \tag{1}$$

between old tuples of coordinates $(\mu) = (x, y, z, \dots)$, and new tuples of coordinates $(\mu') = (x', y', z', \dots)$ in d dimensions. This description is very general, and not necessary to be understood, but describes general steps for performing coordinate transformations, of identifying coordinate functions to represent the relationships between individual coordinates, determining consistent basis unit vectors for the transformed coordinates in terms of the distance vector, and determining components of vectors and gradients in transformed coordinates. Examples for specific coordinate systems are below.

Here, arbitrary individual coordinates from the d-length tuples (μ) or (μ'), are denoted with letters $\mu, \nu, \dots$ or $\mu', \nu', \dots$. Basis vectors from the set of d coordinate basis vectors $\{\vec{\mu}\}$ or $\{\vec{\mu}'\}$, are denoted as $\vec{\mu}, \vec{\nu}, \dots$ or $\vec{\mu}', \vec{\nu}', \dots$. Unless denoted explicitly, arguments to functions $f(\mu)$ are assumed to be functions of all coordinates (old (μ) or new (μ'), depending on whether the variables are primed). Partial derivatives with respect to specific coordinates are denoted by $\partial_\mu = \partial/\partial\mu$. Finally sums over all d coordinates in the tuple are denoted as $\sum_\mu = \sum_{\mu \in \{x,y,z,\dots\}}$.

When considering the basis unit vectors $\{\hat{\mu}\}$ or $\{\hat{\mu}'\}$, it is important to know whether these vectors depend on position, and therefore derivates of any such vectors with respect to the coordinates, must include *derivatives of the unit vectors themselves*. We will assume the old coordinates are *standard*, or *Cartesian* coordinates, such that their unit vectors are *position-independent*, and the new coordinates are generally assumed to be *position-dependent*, such that

$$\partial_\nu \hat{\mu} = 0 \quad , \quad \partial_{\nu'} \hat{\mu}' \neq 0 \ . \tag{2}$$

We may define the coordinate transformations $\mu \to \mu'$ in terms of functions for each coordinate. Each old coordinate, is a function of the new coordinates

$$\mu = f_\mu(\nu') \ , \tag{3}$$

or inversely, each new coordinate, is a function of the old coordinates

$$\mu' = f_{\mu'}(\nu) \ . \tag{4}$$

Let the distance vector $\vec{l}$ be written in the old (standard) basis as

$$\vec{l} = \sum_\mu f_\mu \ \hat{\mu} \tag{5}$$

and therefore the differential distance vector may be written in terms of the new basis differentials as

$$d\vec{l} = \sum_{\mu'} \partial_{\mu'} \vec{l} \, d\mu' \ . \tag{6}$$

The new basis vectors may then be defined as the derivates of the distance vector with respect to each new coordinate

$$\vec{\mu}' = \partial_{\mu'} \vec{l} = \sum_{\nu} \partial_{\mu'} f_\nu \ \hat{\nu} \tag{7}$$

with magnitude

$$\varphi_{\mu'} = |\vec{\mu}'| = \sqrt{\sum_{\nu} |\partial_{\mu'} f_\nu|^2} \ . \tag{8}$$

From these unit vectors in the new coordinate system, the overlap components of the unit vectors in each coordinate system are

$$\hat{\nu}' \cdot \hat{\mu} = \frac{1}{\varphi_{\nu'}} \partial_{\nu'} f_\mu \ , \tag{9}$$

and therefore the basis unit vectors in the old or new coordinates may be expressed in terms of the other coordinates as

$$\hat{\mu}' = \sum_{\nu} \frac{1}{\varphi_{\mu'}} \partial_{\mu'} f_\nu \ \hat{\nu} \tag{10}$$

$$\hat{\mu} = \sum_{\nu'} \frac{1}{\varphi_{\nu'}} \partial_{\nu'} f_\mu \ \hat{\nu}' \ . \tag{11}$$

After performing coordinate transformations, we generally want to express other vectors, and gradients in terms of the new coordinates. Old components a_μ of vectors $\vec{a}$ may be expressed in terms of new components $a_{\mu'}$ with the change of variables

$$a_\mu = \sum_{\nu'} \frac{1}{\varphi_{\nu'}} \partial_{\nu'} f_\mu a_{\nu'} \ . \tag{12}$$

Old derivatives ∂_μ of gradients ∇ may be expressed in terms of new derivatives $\partial_{\mu'}$ with the chain rule

$$\partial_\mu = \sum_{\nu'} \partial_\mu f_{\nu'} \partial_{\nu'} \ . \tag{13}$$

Vectors $\vec{a}$ and gradients ∇ may be expressed as sums of components in any coordinate system

$$\vec{a} = \sum_{\mu} a_\mu \hat{\mu} = \sum_{\mu'} a_{\mu'} \hat{\mu}' = \sum_{\mu,\nu'} \frac{1}{\varphi_{\nu'}} \partial_{\nu'} f_\mu a_{\nu'} \hat{\mu} \tag{14}$$

$$\nabla = \sum_{\mu} \hat{\mu} \partial_\mu = \sum_{\mu'} \hat{\mu}' \frac{1}{\varphi_{\mu'}} \partial_{\mu'} = \sum_{\mu,\nu'} \hat{\mu} \partial_\mu f_{\nu'} \partial_{\nu'} \ . \tag{15}$$

Notice how the vectors and gradients transform inversely to each other, with vectors being transformed in terms of the old coordinate functions f_μ, and the gradients being transformed in terms of the new coordinate functions $f_{\mu'}$. In general, quantities, that appear in the old coordinate system as simple dot products between gradients and vectors, due to standard basis vectors being position independent, now have additional terms due to the new basis vectors being position dependent.

For example, the divergence of a vector $\vec{a}$ in the new coordinate system is

$$\nabla \cdot \vec{a} = \sum_\mu \partial_\mu a_\mu = \sum_\mu \left[\sum_{\nu'} \partial_\mu f_{\nu'} \partial_{\nu'}\right] \left[\sum_{\eta'} \frac{1}{\varphi_{\eta'}} \partial_{\eta'} f_\mu a_{\eta'}\right] . \tag{16}$$

1.2 Polar Coordinates

Let us consider $d = 2$ transformation between old Cartesian and new Polar coordinates

$$(x, y) \to (s, \phi) . \tag{17}$$

Our general procedure is as follows to derive quantities in terms of new coordinates, including unit vectors, vector components, and gradient partial derivatives:

1. Derive the distance vector $\vec{l} = x\hat{x} + y\hat{y}$ in terms of the new coordinates, given we know $x = f_x(s, \phi)$, $y = f_y(s, \phi)$, or equivalently $s = f_s(x, y)$, $\phi = f_\phi(x, y)$ for some functions for each coordinate, depending on the specific transformation.

2. Derive the new coordinate unit basis vectors $\hat{s}, \hat{\phi}$ in terms of the old coordinate unit basis vectors $\hat{x}, \hat{y}$, given (non-unit) basis vectors are defined as $\vec{s} = \frac{\partial \vec{l}}{\partial s}$, $\vec{\phi} = \frac{\partial \vec{l}}{\partial \phi}$.

3. Derive vector $\vec{a}$ old coordinate components a_x, a_y in terms of new coordinate components a_s, a_ϕ, given all vectors can be expressed as sums of orthogonal components in any coordinates $\vec{a} = a_x\hat{x} + a_y\hat{y} = a_s\hat{s} + a_\phi\hat{\phi}$.

4. Derive gradient partial derivatives with respect to old coordinates in terms of partial derivatives with respect to new coordinate, given the chain rule, and that the new coordinates depend the old coordinates,
$\frac{\partial}{\partial x} = \frac{\partial s}{\partial x}\frac{\partial}{\partial s} + \frac{\partial \phi}{\partial x}\frac{\partial}{\partial \phi} = \frac{\partial f_s(x,y)}{\partial x}\frac{\partial}{\partial s} + \frac{\partial f_\phi(x,y)}{\partial x}\frac{\partial}{\partial \phi}$, $\frac{\partial}{\partial y} = \frac{\partial s}{\partial y}\frac{\partial}{\partial s} + \frac{\partial \phi}{\partial y}\frac{\partial}{\partial \phi} = \frac{\partial f_s(x,y)}{\partial y}\frac{\partial}{\partial s} + \frac{\partial f_\phi(x,y)}{\partial y}\frac{\partial}{\partial \phi}$.

5. Derive quantities of interest in new coordinates, given known equations involving old coordinates, (such as the divergence $\nabla \cdot \vec{a} = \frac{\partial}{\partial x} a_x + \frac{\partial}{\partial y} a_y$), given we know now the partial derivatives and the vector components, written in the old coordinates, in terms of the new coordinates.

The associated coordinate transformation functions are

$$x = s\cos(\phi) \quad , \quad y = s\sin(\phi) \tag{18}$$

$$s = \sqrt{x^2+y^2} \quad , \quad \phi = \tan^{-1}\frac{y}{x} \ . \tag{19}$$

The distance vector is

$$\vec{l} = s\cos(\phi)\hat{x} + s\sin(\phi)\hat{y} \tag{20}$$

$$d\vec{l} = \ (\cos(\phi)\hat{x} + \sin(\phi)\hat{y})\, ds \ + \ (-s\sin(\phi)\hat{x} + s\cos(\phi)\hat{y})\, d\phi \ . \tag{21}$$

The new basis vectors are

$$\vec{s} = \cos(\phi)\hat{x} + \sin(\phi)\hat{y} \quad , \quad \vec{\phi} = -s\sin(\phi)\hat{x} + s\cos(\phi)\hat{y} \tag{22}$$

$$\varphi_s = 1 \quad , \quad \varphi_\phi = s \tag{23}$$

$$\hat{s} = \cos(\phi)\hat{x} + \sin(\phi)\hat{y} \quad , \quad \vec{\phi} = -\sin(\phi)\hat{x} + \cos(\phi)\hat{y} \ . \tag{24}$$

Therefore the distance vector may be expressed as

$$\vec{l} = s\hat{s} \tag{25}$$

$$d\vec{l} = ds\hat{s} + sd\phi\hat{\phi} \ . \tag{26}$$

The components between new and old basis unit vectors are

$$\hat{x}\cdot\hat{s} = \cos(\phi) \quad , \quad \hat{y}\cdot\hat{s} = \sin(\phi) \tag{27}$$

$$\hat{x}\cdot\hat{\phi} = -\sin(\phi) \quad , \quad \hat{y}\cdot\hat{\phi} = \cos(\phi) \ . \tag{28}$$

The old basis unit vectors are

$$\hat{x} = \cos(\phi)\hat{s} - \sin(\phi)\hat{\phi} \quad , \quad \hat{y} = \sin(\phi)\hat{s} + \cos(\phi)\hat{\phi} \ . \tag{29}$$

Vectors with old components expressed in the new components are

$$a_x = \cos(\phi)a_s - \sin(\phi)a_\phi \quad , \quad a_y = \sin(\phi)a_s + \cos(\phi)a_\phi \ . \tag{30}$$

Gradients with old derivatives expressed in the new derivatives are

$$\partial_x = \cos(\phi)\partial_s - \frac{1}{s}\sin(\phi)\partial_\phi \quad , \quad \partial_x = \sin(\phi)\partial_s + \frac{1}{s}\cos(\phi)\partial_\phi \ . \tag{31}$$

The divergence in new components is

$$\begin{aligned}\nabla\cdot\vec{a} = &\ \left(\cos(\phi)\partial_s - \frac{1}{s}\sin(\phi)\partial_\phi\right)\left(a_s\cos(\phi) - a_\phi\sin(\phi)\right) \ + \\ &\left(\sin(\phi)\partial_s + \frac{1}{s}\cos(\phi)\partial_\phi\right)\left(a_s\sin(\phi) + a_\phi\cos(\phi)\right)\end{aligned} \tag{32}$$

$$\nabla\cdot\vec{a} = \frac{1}{s}\partial_s\left(sa_s\right) \ + \ \frac{1}{s}\partial_\phi\left(a_\phi\right) \ . \tag{33}$$

PHYS242 - Assignment and Exam Questions

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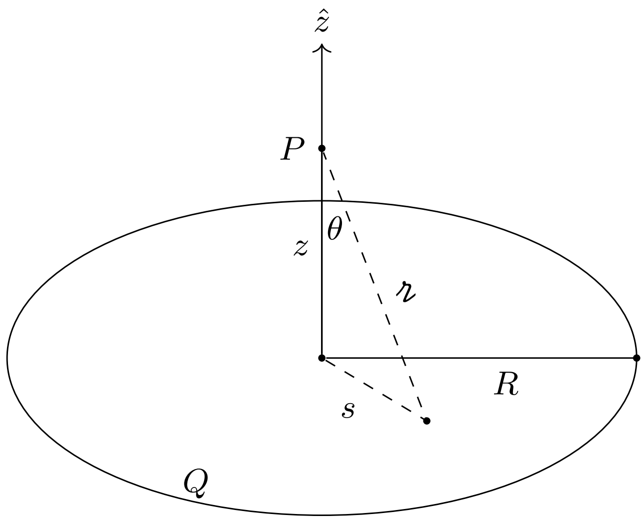
I. ELECTROSTATICS

1. **Electric Field of Solid Disk**
   Imagine you are at a point P, and are near a uniformly charged solid disk (with no thickness, but charged throughout its area), of radius R, and total charge Q.



   (a) What are the non-zero components of the field $\vec{E}$ in cylindrical coordinates if P is centred along the axis of the disk, from symmetry arguments? (Explain about each component of the field and its dependence on each coordinate.)

   Solution:
   At an arbitrary point P, not necessarily along the axis of the disk at $s = 0$, there will be radial s and height z dependence, depending on the point's position relative to the disk, however due to the disk being uniform and looking identical no matter from which angular it is observed, there will be no angular dependence. Specifically along the axis of the disk at $s = 0$, there will be additional radial symmetry. Therefore at an arbitrary point P:
   From the angular symmetry of the disk, $E_\phi = 0$, due to $E_\phi(s, z, \phi) = -E_\phi(z, s, \pi + \phi) = -E_\phi(z, s, \phi) = 0$. From the position of P, $E_s = E_s(z, s) \neq 0$, due to there being no radial symmetries. From the position of P, $E_z = E_z(z, s) \neq 0$, due to there being no z symmetries.

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(b) What is the electric field $\vec{E}$ due to the disk, if $p = z$ is a distance z above the plane of the disk, centred at the origin?

Solution:
Let the disk area element be $dS = s ds d\phi$, *for* $s \in [0, R]$, $\phi \in [0, 2\pi]$, *let the radial position from* P *be* $\mathscr{r}^2 = z^2 + s^2$, *let the azimuthal angle from* P *be* θ *such that* $\tan\theta = s/z$, *and let the surface charge density be* $\sigma = Q/S$, *where* $S = \pi R^2$. *Given the polar angular symmetry* $\phi \in [0, 2\pi]$, *we will change variables and express the radial coordinate* $s \in [0, R]$ *in terms of the positional distance coordinate* $\mathscr{r} \in [|z|, \sqrt{z^2 + R^2}]$, *where* $\mathscr{r} d\mathscr{r} = s ds$, *and therefore* $dS = 2\pi \mathscr{r} d\mathscr{r}$, *and positional vector* $\hat{\mathscr{r}} = (z/\mathscr{r})\hat{z} + (s/\mathscr{r})\hat{s}$. *By symmetry of the radial components cancelling over the integration, only the* $\hat{z}$ *component must be integrated over, and* $\vec{E} = E_z(z)\hat{z}$. *Therefore the electric field element is*

$$d\vec{E} = \frac{1}{4\pi\epsilon_0} dS \frac{\sigma}{\mathscr{r}^2} = 2\pi \frac{1}{4\pi\epsilon_0} \frac{Q}{\pi R^2} z\hat{z} \; d\mathscr{r} \frac{1}{\mathscr{r}^2} \ , \tag{1}$$

$$\vec{E} = \int d\vec{E} = 2\pi \frac{1}{4\pi\epsilon_0} \frac{Q}{\pi R^2} \; z\hat{z} \; \int_{|z|}^{\sqrt{z^2+R^2}} d\mathscr{r} \; \frac{1}{\mathscr{r}^2} \ , \tag{2}$$

and therefore the total electric field is

$$\vec{E} = 2 \frac{1}{4\pi\epsilon_0} \frac{Q}{R^2} \left[1 - \frac{1}{\sqrt{1 + (R/z)^2}} \right] \hat{z} \ . \tag{3}$$

(c) What is the electric field $\vec{E}$ due to the disk, if P is very far from the disk? What if P is very close to the disk?

Solution:
Given $1/\sqrt{1 + x^2} = 1 - (1/2)x^2 + O(x^3)$ *for* $x \ll 1$, *and* $1/\sqrt{1 + x^2} = 1$ *for* $x \gg 1$, *the following limits hold*

$$\lim_{z \to \infty} \vec{E} = \frac{1}{4\pi\epsilon_0} \frac{Q}{z^2} \hat{z} \tag{4}$$

$$\lim_{z \to 0} \vec{E} = \frac{\sigma}{2\epsilon_0} \hat{z} \ . \tag{5}$$

and in the limit of being close to the disk $z \ll R$, *the constant, infinite plane electric field is recovered, and in the limit of being far from the disk* $z \gg R$, *the* $1/R^2$ *point charge electric field is recovered.*

(d) What is the electric field $\vec{E}$ due to the disk, if P is not centred at the origin of the disk? (Setup equations and explain difficulties of exact solutions.)

Solution:
In the case of P *not being centred at the origin, there is still angular symmetry due to the disk geometry being angularly symmetric, however the electric field will generally have non-zero* z *and radial components* $E_z = E_z(z, s)$, $E_s = E_s(z, s)$. *Further, the simplest integration variables will be complicated due to the radial offset of the point by* t. *This leads to electric fields of the form*

$$\vec{E} = 2 \frac{1}{2\pi} \frac{1}{4\pi\epsilon_0} \frac{Q}{R^2} \quad \int_0^R \int_0^{2\pi} ds \; d\phi \; \frac{s}{\left(z^2 + s^2 + t^2 - 2ts\hat{t} \cdot \hat{s}\right)^{3/2}} \left[z\hat{z} + t\hat{t} - s\hat{s} \right] \ , \tag{6}$$

which has no closed form solution, however can be expressed in terms of elliptical integrals.

(e) What is the electric field outside and inside of the disk, if the disk has a non-zero thickness h and uniform charge density ρ? (Explain difficulties of exact solutions.) What if the disk becomes an infinitely long cylinder $h \to \infty$? *In the case of the disk having a finite thickness* h, *there are significant edge effects, where the accumulation of charges along the edges of the disk cause electric fields pointing outwards, not just transversally in the* $\hat{z}$ *direction upwards, but also laterally in the* $\hat{s}$ *direction away from the disk.*
In the case of the disk becoming an infinitely long cylinder, the dominant electric field switches from being in the transversal $\hat{z}$ *direction to the lateral* $\hat{s}$ *direction, and by symmetry, Gauss' law can be used*

$$\vec{E} = \frac{1}{2} \frac{1}{\epsilon_0} \rho \begin{cases} s & s \leq R \\ \frac{R^2}{s} & s \geq R \end{cases} \hat{s} \tag{7}$$

2. **Dipole Moment of Circle of Charges**
Imagine you are at the centre of circle of radius r, and there are n charges $\{q_k = (q/n)\cos\theta_k \ : \ \theta_k = k\theta^{(n)}\ ,\ \theta^{(n)} = 2\pi/n\}_{k=0}^{n-1}$, evenly distributed on a circle.

   (a) What is the dipole moment of these charges?

   Solution:
   From the definition of the dipole moment $\vec{p} = \sum_q q\ \vec{r}_q$, and using that $\sum_k^n e^{-ijk\theta^{(n)}} = n\delta_{j0}$, the dipole moment of the discrete charges is

$$\vec{p} = \sum_k^n \left[\frac{q}{n}\cos\theta_k\right]\left[r\cos\theta_k\hat{x}\ +\ r\sin\theta_k\hat{y}\right] \tag{8}$$

$$= \frac{qr}{2}\frac{1}{n}\sum_k^n (1+\cos 2\theta_k)\hat{x}\ +\ (\sin 2\theta_k)\hat{y} \tag{9}$$

$$= \frac{qr}{2}\hat{x}\ . \tag{10}$$

   (b) What is the dipole moment of these charges if $n \to \infty$ and you have a continuous line density of charges $\lambda(\theta) = (q/2\pi r)\cos\theta$ along the circle?

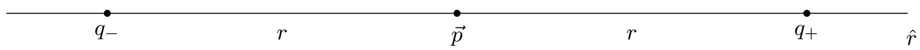
   Solution:
   From the definition of the dipole moment $\vec{p} = \int dq\ \vec{r}(q)$, and using that $\int_0^{2\pi} d\theta\ e^{-ij\theta} = 2\pi\delta_{j0}$, the dipole moment of the continuous charges is

$$\vec{p} = \int_0^{2\pi} d\theta\ \left[\frac{q}{2\pi}\cos\theta\right]\left[r\cos\theta\hat{x}\ +\ r\sin\theta\hat{y}\right] \tag{11}$$

$$= \frac{qr}{2}\frac{1}{2\pi}\int_0^{2\pi} d\theta\ (1+\cos 2\theta)\hat{x}\ +\ (\sin 2\theta)\hat{y} \tag{12}$$

$$= \frac{qr}{2}\hat{x}\ . \tag{13}$$

3. **Force and Torque with Dipoles**
Imagine you have an electric dipole $\vec{p}$ at the origin, and along an axis $\hat{r}$ there are 2 point changes $q_{\pm}$ a distance $\pm r\hat{r}$ away. What is the force and torque felt by the dipole? How do your answers change if $q_+ = -q_- = -q$, and the dipole $\vec{p}$ is parallel or perpendicular to the axis $\hat{r}$? What if $q_+ = q_- = q$?



The force $\vec{F}$ and torque $\vec{T}$ on dipoles $\vec{p}$ due to an electric field $\vec{E}$ are

$$\vec{F} = \vec{p} \cdot \nabla \vec{E} \tag{14}$$

$$\vec{T} = \vec{p} \times \vec{E} \ . \tag{15}$$

The vector gradient product $\vec{a} \cdot \nabla$ of constant direction fields $\vec{b} = f\hat{c}$ for constant $\vec{c}$ is

$$(\vec{a} \cdot \nabla) f\hat{c} = (\vec{a} \cdot \nabla f)\hat{c} \ , \tag{16}$$

the vector gradient product $\vec{a} \cdot \nabla$ of radial fields $\vec{b} = f\hat{r}$ for $f = f(r)$ is

$$(\vec{a} \cdot \nabla) f\hat{r} = \frac{f\vec{a} - \vec{a} \cdot (f\hat{r} - r\nabla f)\hat{r}}{r} \ . \tag{17}$$

For radial functions $f(r) = 1/r^\alpha$ for constant powers $\alpha \geq 0$,

$$\nabla \frac{1}{r^\alpha} = -\alpha \frac{1}{r} \frac{1}{r^\alpha} \hat{r} \ , \tag{18}$$

leading to the vector gradient product

$$(\vec{a} \cdot \nabla) \frac{1}{r^\alpha} \hat{r} = \frac{\vec{a} - (\alpha + 1)\vec{a} \cdot \hat{r} \ \hat{r}}{r^{\alpha+1}} \ . \tag{19}$$

Given the point charges have electric fields at the dipole of

$$\vec{E} = -\frac{1}{4\pi\epsilon_0} \frac{q_+ - q_-}{r^2} \hat{r} \ , \tag{20}$$

therefore the force and torque on a dipole are

$$\vec{F} = -\frac{1}{4\pi\epsilon_0} \frac{q_+ - q_-}{r^3} \left[\vec{p} - 3\vec{p} \cdot \hat{r} \ \hat{r}\right] \tag{21}$$

$$\vec{T} = -\frac{1}{4\pi\epsilon_0} \frac{q_+ - q_-}{r^2} \ \vec{p} \times \hat{r} \ . \tag{22}$$

If $q_+ = -q_- = -q$, and the dipole is parallel to the axis $\vec{p} \parallel \hat{r}$

$$\vec{F} = 2(3-1) \frac{1}{4\pi\epsilon_0} \frac{q}{r^3} \vec{p} \tag{23}$$

$$\vec{T} = 0 \ . \tag{24}$$

If $q_+ = -q_- = -q$, and the dipole is perpendicular to the axis $\vec{p} \perp \hat{r}$

$$\vec{F} = 2 \frac{1}{4\pi\epsilon_0} \frac{q}{r^3} \vec{p} \tag{25}$$

$$\vec{T} = 2p \frac{1}{4\pi\epsilon_0} \frac{q}{r^2} \ \hat{p} \times \hat{r} \ . \tag{26}$$

If $q_+ = q_- = q$,

$$\vec{F} = 0 \tag{27}$$

$$\vec{T} = 0 \ . \tag{28}$$

ISSYP 2022 Mentoring

What is magnetism and what does it tell us about phases of matter?

Session 2 - Phases of Matter and Lattice Models

July 26, 2022

Abstract

In Session 2, we discuss the concept of phases of matter in materials around us, and discuss similarities and differences between both different phases, and different materials which exhibit different types of phases of matter. We then discuss how we could approach modelling these phases of matter using mathematics, and the language of statistical physics. We finally introduce an important playground for modelling materials, and investigating phases of matter, that of discrete lattices of sites, connected by bonds. These lattices offer an intuitive background for proposing statistical models, and we discuss examples of lattices, and how they can be used to visualize interactions between constituents in a material.

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1 What are Phases of Matter?

What do we think of when we talk about phases of matter?

There are many materials around us, all made up of basic building block constituents, depending how far we zoom in, they could be molecules, or atoms, or even sub-atomic particles. Each material has some unique characteristics, but we can further categorize them by what *phase* they are in, and there are usually *universal* characteristics of each phase across a wide range of materials. An important direction in physics is understanding how to classify these phases of matter, and determining how to best characterize these universal phenomena.

1.1 Distinguishing Phases of Matter

What distinguishes phases of matter? What could we measure to determine which phase a material is in?

What are some universal characteristics of solid, liquid, and gas phases across different materials? What distinguishes the materials?

1.2 Phase Transitions

Arguably more important than identifying phases of matter, is understanding how they *transition* from one phase, and what environmental factors *drive* these transitions.

What property of the environment forces water to be in one of its phases?

How could we write mathematically the presence of a phase transition in a particular quantity?

Phases of matter, and phase transitions are somewhat intuitive, however are notoriously difficult to describe mathematically. We will now present several aspects of modelling materials that will help towards obtaining a complete physical and mathematical description of phases of materials.

Why are phase transitions difficult to describe mathematically?

Phase transitions arise when there is an *abrupt* change in some important quantity called an *order-parameter* (i.e) the *density* and configuration of particles in water), when certain independent parameters exceeds certain *critical values* (i.e) the freezing or boiling *temperature* of water). Ideally, these abrupt changes of quantities result in very different macroscopic properties of the material, that we can identify as being in very different phases (i.e) liquid and solid water have very different properties).

We can model this mathematically by first finding a suitable quantity of interest, that from our physical intuition, appears to possibly change as another parameter changes past a certain point, and then study the *dependence* of these variables. Most behaviours in physics and materials tend to change *smoothly* (i.e) plastics slowly deform when stressed, and don't spontaneously change to some fundamentally different material), and so these abrupt changes can be difficult to conceptualize and describe mathematically.

For complicated systems, it can be difficult and not at all obvious whether there are phases and phase transitions, and which quantities are most appropriate to indicate these phase transitions. Fortunately, as we will discuss throughout these sessions, many materials behave very similarly at a fundamental level, and there are underlying phenomena that cause the existence of similar phase transitions across these different materials.

We have seen that the *Temperature*, and its scale relative to the energy of a system affects the Boltzmann distribution for how likely a material is to have a certain amount of energy. Temperature is in fact often the driving factor that causes phase transitions at a certain *critical-temperature*.

2 Models of Materials

As physicists, we must develop what are known as *models* of materials. These models are mathematical descriptions for how basic constituents of a material, what physicists call *particles*, evolve over time, and interact with each other. In order to start developing these models, and approaches for extracting important properties about the material using calculations, we must first develop some intuition behind how these particles may *interact*, how we can describe the *environment* the particles occupy, and some governing *principles* that dictate how these particles evolve and reach some kind of equilibrium over time.

What are different interactions between particles that you can think of? Hint: Think about electromagnetic and gravitational forces

Imagine we have a particle that can be in one of two states: $\sigma = \pm 1$ *and* $\Xi = \{\pm 1\}$*, a so-called* two-level system. *How could we represent this state mathematically? How could we write down an interaction between two of these particles?*

Imagine we have now a set of N *of these particles* $\sigma = \{\sigma_i = \pm 1 \; : \; i = 1 \cdots N\}$*, and* $\Xi = (\Xi_1, \Xi_2, \ldots, \Xi_N)$*, where* $\Xi_i = \{\pm 1\}$*. What would be some intuitive and simple ways of arranging these particles, that intuitively shows and constrains which particles interact most with which (*Hint: Nearby*) particles?*

2.1 Calculations based on Models

When we talk of forming mathematical models of materials, we must also talk about performing *calculations* with these models. Calculating generally refers to extracting useful, intuitive, and *experimentally-relevant* quantities about the materials being described. Some examples could be the heat capacity: how much heat is required to raise a material's temperature, or its bulk modulus: how much its volume changes when pressure is applied, or its magnetic susceptibility: how much magnetic field it gives off when exposed to a magnetic field. One way of calculating these quantities, is to assume that the system has some randomness, and can be in different configurations σ that have an *energy* ε_σ. When it is at a fixed temperature T in equilibrium with its environment, it follows the *Boltzmann* distribution

$$p_\sigma = \frac{1}{Z} e^{-\frac{\varepsilon_\sigma}{T}} \tag{1}$$

where $Z = \sum_{\sigma \in \Xi} e^{-\frac{\varepsilon_\sigma}{T}}$ is the probability normalization factor as the sum over all possible configurations, or (micro)states that the system can be in. To calculate f_σ, that are assumed to be functions of which state the system is in, this amounts to estimating the *expectation value* of these quantities, over this distribution of possible energetic states

$$\langle f \rangle = \sum_{\sigma \in \Xi} p_\sigma f_\sigma \; . \tag{2}$$

How could we write $\langle f \rangle$ *as a function of solely the partition function?*

3 Concept of Energy in a System

The concept of energy can be abstract, and what do we mean by the energy $\varepsilon = \varepsilon_\sigma$ of a system for a configuration σ? We have probably seen that materials with mass m can have kinetic energy from being in motion with speed v, $\varepsilon_v = v^2/2m$, or gravitational potential energy from being at a height z, $\varepsilon_z = mgz$, or electromagnetic energy from being attracted or repelled from a particle with charge e a distance r away, $\varepsilon_r = -e/4\pi\varepsilon_0 r$. When concerned with the dynamics, or kinematics of a system, we can think of the *forces* acting on particles, causing their motion, or we can equally think about the energy that particles have as they move around, and eventually lose, or gain energy, depending how they collide, or interact with other particles.

How would we describe the total energy of a system of N such particles, each with the energies above?

Energy is essentially a *local* quantity, meaning it can generally be written as a sum over the energy ε_i of each separate particle i, which includes energy that a particle has, plus energy that it possesses from interacting with other particles. Energy can thus be written as a sum over each of N particles

$$\varepsilon_\sigma = \sum_i^N \varepsilon_{\sigma_i} \ . \tag{3}$$

What governing principle do systems with a defined energy obey? Hint: Do systems want to be in high energy, or low energy states?

Due to the Boltzmann equation having the form of an exponential of the energy, how are the probabilities affected if all energies are shifted *by a* constant *energy value?*

3.1 Interaction Energies

Given we can describe the energies, of individual particles, we must now supplement our energy description with the energy representing how particles interact. By the principle of energy minimization, interactions that are favoured, such as gravitational attraction between massive particles, will *decrease* the energy, whereas interactions that are not favoured, such as electromagnetic attraction between equally charged particles, will *increase* the energy.

4 Lattices

Given these notions of the states that particles can be in, the interactions between particles, and this concept of energies of a system of particles, the last important aspect of describing models of materials, is the environment that these particles are occupying. A convenient description when dealing with fixed particles, in nice, uniform systems, are grids of sites where these particles live, called *lattices*.

What are lattices? How can we picture them, and describe them mathematically?

Lattices can be described by a set of sites $\Lambda = \{i \ : \ i = 1 \cdots N\}$, connected by bonds $\Delta = \{\delta = (i, j) \ : \ i, j \in \Lambda\}$. For example, we could have a lattice that is *symmetrical*, or *translationally invariant*, with all sites having the same *coordination number*, or number of nearest-neighbour bonds z. Examples of these lattice, are the *square*, *triangular*, or *hexagonal* lattices.

How many nearest-neighbours does each of the square*,* triangular*, or* hexagonal *lattices have?*

4.1 Performing summations on Lattices

We often come across summations over the sites and bonds of a lattice in models of interactions between particles that are arranged on a lattice. Performing the correct combinatorics of counting these numbers of sites and bonds, and keeping track of the symmetries present in the lattice is an important skill.

For example, if we are summing over all sites in a lattice, we often denote this for functions of a site f_i as

$$\sum_i f_i \ , \tag{4}$$

whereas if we are summing over all nearest-neighbour bonds in a lattice, we often denote this for functions of a bond f_{ij} as

$$\sum_{<ij>} f_{ij} \ , \tag{5}$$

and we can also denote this as a summation over all lattice sites, and each sites' nearest-neighbours

$$\sum_{<ij>} f_{ij} = \frac{1}{2} \sum_i \sum_{<ji>} f_{ij} \ , \tag{6}$$

and denote all nearest neighbours of site i as $< ji >$, or just $< i >$.

Why is there the factor of $1/2$ *when initially summing over all lattice sites, then nearest-*

neighbours?

How might we perform this summation where functions f_i are of sites,

$$\sum_{<ij>} f_i + f_j \tag{7}$$

for a lattice with N sites, and constant coordination number z?

4.2 Homogeneity in Lattices

Depending on the system that is being modelling on the lattice, and the quantities being calculated, the system may be *homogenous*, meaning all sites are essentially identical, and a particle at one site is *indistinguishable* from a particle at another site. We can also discuss taking what is known as the *thermodynamic limit* of the lattice, where the number of particles

$$N \to \infty \tag{8}$$

to represent realistic systems with at least an Avogadro's number of particles.

Lattices can also be in spaces of different numbers of *spatial dimension* d. We live in $d = 3$ dimensions, but could also look at a $d = 1$ dimensional *chain* of sites, or a $d = 2$ dimensional *plane* of sites, or even a more abstract $d > 3$ dimensional *hyper-lattice* of sites.

How does the dimensionality of the lattice affect the coordination number? Enumerate the nearest-neighbours in d dimensions for a hyper-cubic lattice.

5 Lattice Models of Magnetism

Now that we have a sense of some interactions between some 2-level particles, and the lattices that these particles may live on, how may we define a model that represents this system? This concept of energy ε, and the principle of energy minimization, is very general, and offers an intuitive framework for modelling the present state of a system by how much energy it possesses. Given a system will tend towards it lowest energy configuration, this energetic description indicates how the system will evolve towards this state. One important method of modelling a system therefore consists of determining an accurate, but as simple as possible, mathematical description of the energy of a system of particles. We also want to develop models that are as *general* as possible, and serve to describe as many materials and systems as possible, so as to determine the most fundamental underlying phenomena that govern many materials, and to avoid having to develop a new model each time we encounter a new material.

5.1 Ising Model of Magnetism

We will start, perhaps not intuitively, with the most fundamental model of magnetism, the *Ising* model. It will seem incredibly simple at first, but throughout our analysis, we will slowly begin to see its subtleties, and how all of its features, and intuition that we gain from it, will show up constantly in any more sophisticated models that we subsequently analyse. Furthermore, even though it is initially posed as a model for magnetism, the fact it is a 2-level system, means other systems where particles can be in one of two states, can be translated, or *mapped*, into a form that resembles the Ising model. This concept of *mapping* one description of a system, usually one that appears very complicated, and difficult to perform calculations with, to a related system that we already have intuition, or calculated results about, is an essential part of physical modelling as well.

Let us now define the Ising particles $\sigma_i = \pm 1$ as random variables on a lattice of N sites. We can think of each site as being a mini bar-magnet, either pointing up or down.

Each particle only interacts with its z *nearest-neighbours*, with a *ferromagnetic* interaction, meaning the system wants to align all of its nearest-neighbours to point along the same direction, this being the lowest energy state. There also may be an external magnetic field, that the particles will want to *align* themselves with.

How may we write this model?

We can thus write the energy of the Ising model for a given configuration $\sigma = (\sigma_1, \sigma_2, \ldots, \sigma_N)$ of N particles on a lattice as

$$\varepsilon_\sigma = -J \sum_{<ij>} \sigma_i \sigma_j - h \sum_i \sigma_i \tag{9}$$

where J represents how strongly the particles will tend to align with each other, and h represents the strength of the external magnetic field that forces the particles to align along its direction.

What is the local *energy of each particle in the Ising model?*

Notice, that we have not indicated what kind of lattice the particles of this model live on, or which number of *spatial dimensions* we are in. In fact this model is very general, and only requires us to know for each particle and site i, its z nearest-neighbours $< ij >$, and so could potentially model magnetism of particles on any lattice we choose.

Does this model make sense? Why are there minus-signs? How would we write this model for a $d = 1$ dimensional chain of Ising particles?

What is the ground-state *of the* ferromagnetic *Ising model on a* triangular lattice*?*

What if there were no minus signs? What would be the ground-state *of the* anti-ferromagnetic *Ising model on a* triangular lattice*?*

We can think of each Ising particle interacting with each of its nearest-neighbours, and this external field, and please note the *minus-signs*, to represent that it is *energetically-favourable* for the particles to align along these interactions.

Given this model of energy in an Ising model, how does this relate to our previous discussion of the Boltzmann distribution, and most energetically favourable states?

Is there any reason to think there could be different phases for particles following this Ising model?

What could be possible quantities that drive any phase transitions, and what quantities could indicate which phase the particles are in?

For example, we could calculate the average magnetization of each particle

$$\langle \sigma \rangle = \frac{1}{N} \sum_i \left(\sum_{\sigma \in \Xi} p_\sigma \ \sigma_i \right) \ , \tag{10}$$

or the average energy of a lattice per particle

$$\langle \varepsilon \rangle = \frac{1}{N} \sum_i \left(\sum_{\sigma \in \Xi} p_\sigma \ \varepsilon_{\sigma_i} \right) \ , \tag{11}$$

We will see how these quantities arise when determining whether there are phases and phase transitions in our model of magnetism, whether they ever abruptly change, and how temperature affects these quantities.

6 Summary

In this session, we have introduced the concepts of phases of matter, and transitions between these phases, and discussed the difficulties and many concepts required to develop a mathematical description of these phases. We then discussed the process that physicists use to develop models for materials, and kinds of interactions between fundamental constituents, or particles that are being described by these models. We then introduced lattices, and how a particle can occupy each site, and interact through bonds between particles on this lattices, and gained some familiarity with summations over these particles and bonds on the lattice. Finally, we used these concepts to introduce our first model of magnetism, the ferromagnetic Ising model, with nearest-neighbour interactions.

In the next session, we will discuss what it means for a model to be easy or difficult to study. We will study the Ising model further, and introduce an important approach to making predictions based on a model called Mean-Field Theory. We will then start some calculations with this Ising model, using our new mean field theoretic approaches, and start to see how particles following the Ising model could exhibit distinct phases.

Are there any additional questions or comments?

What is everyone taking away from this session?

What would everyone like to learn more about regarding this session?

How was the level of content and delivery of this session?