Title: Symposium Talk

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Collection/Series: Year of Quantum Across Canada

Subject: Quantum Information

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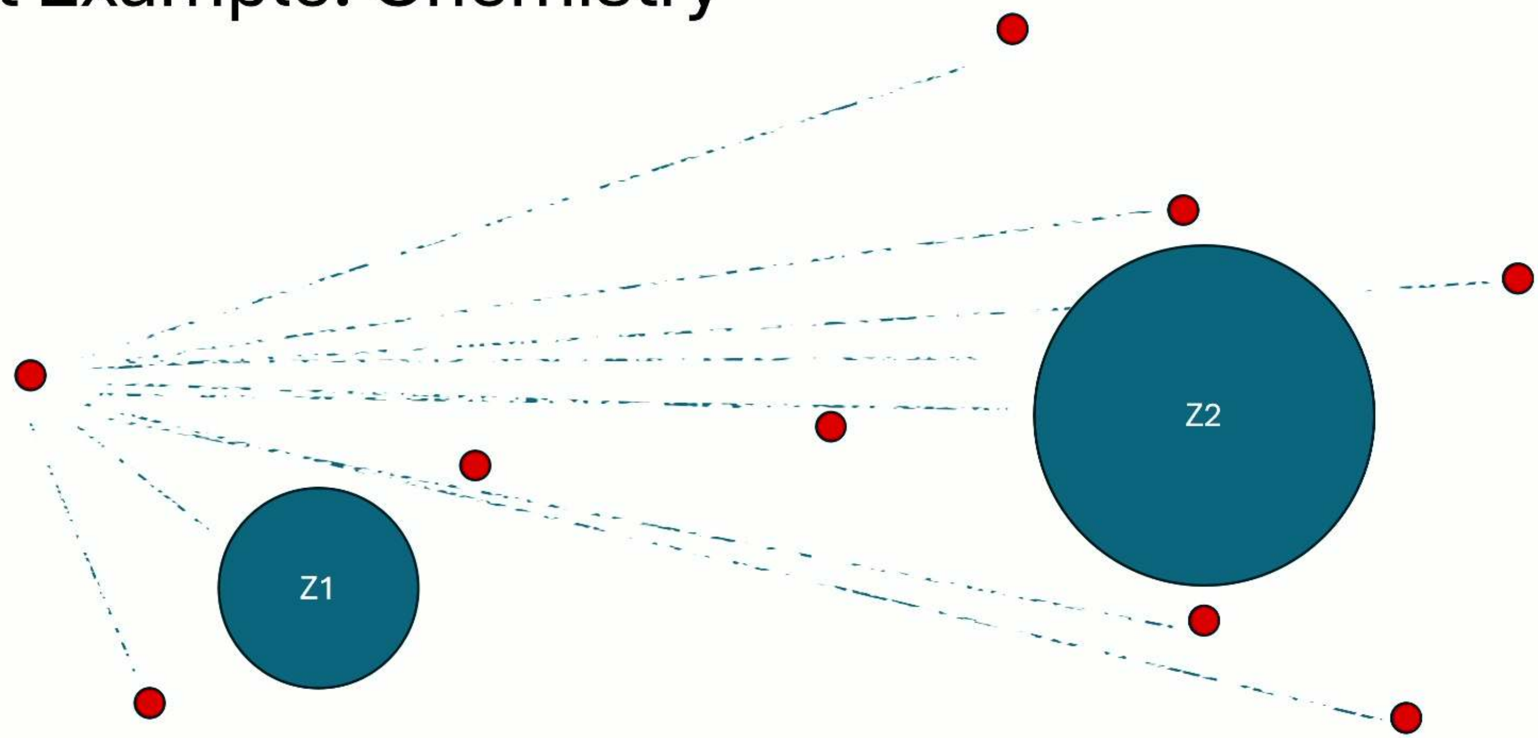
Is Fundamental Physics Fundamentally Simpler?

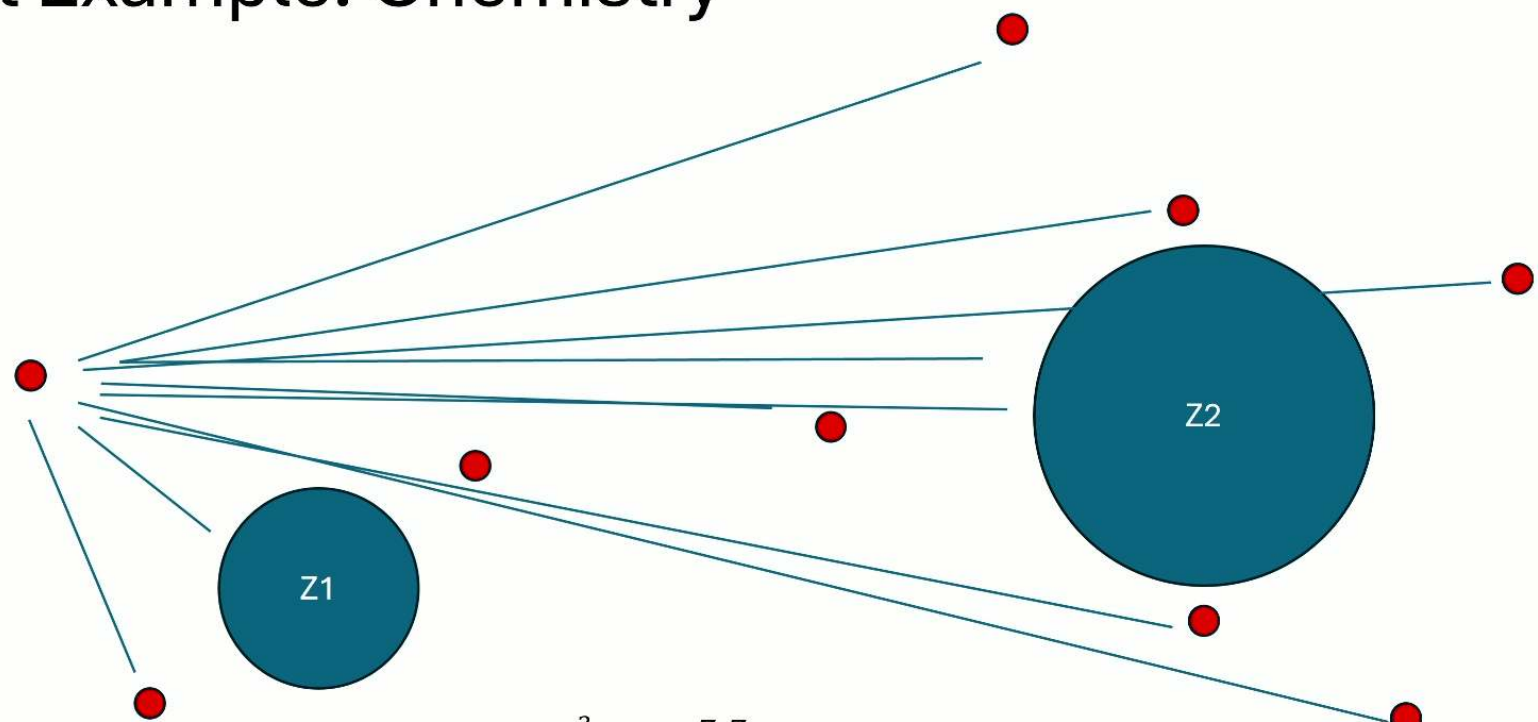
(Boring title: Simulation of Non-Relativistic Quantum Electrodynamics with Topologically Protected Emergent Coulomb Interactions)

Nathan Wiebe

Test Example: Chemistry



Test Example: Chemistry

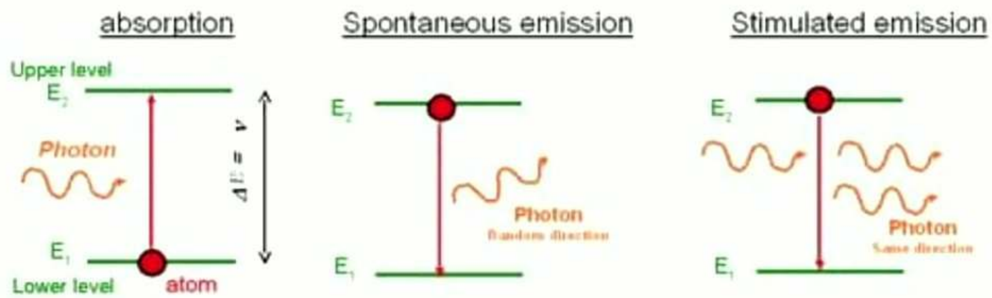


$$H = \sum_i \frac{p^2}{2m_i} + \sum_{i,j} \frac{Z_i Z_j}{r_{ij}}$$

Is this simulation right?

- No there are a bunch of fundamental effects that we ignore

1) No external quantum electromagnetic fields fields
2) Infinit
3) No m



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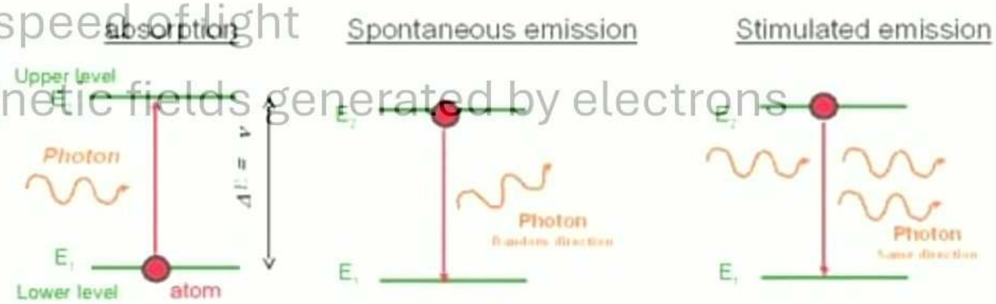

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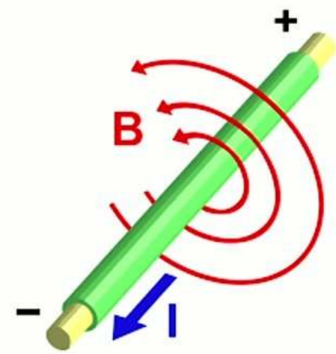


A better model

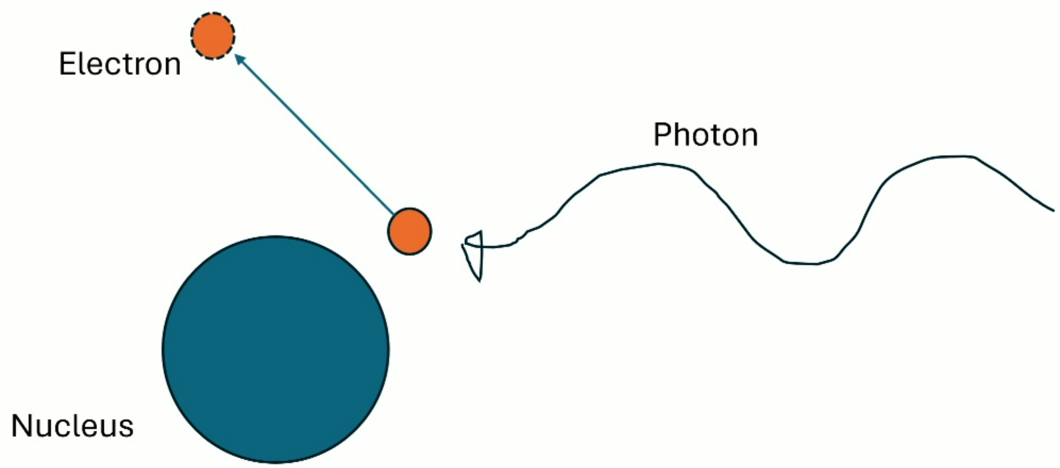
- The Pauli-Fierz model gives a correct treatment of single particle non-relative electrodynamics.
- The model has interactions with a background field and correctly includes both quantum electric and magnetic effects.
- It does NOT deal with multiple particles because the motion of particles does not lead to an updated field.
  - No Ampere's law
  - No Gauss' law

$$\hat{H} = \sum_{j}^{\eta} \left[\left(\mathbf{p}_j - \frac{e}{c}\mathbf{A}(x) \right)^2 - \frac{e}{c}\boldsymbol{\sigma}_j \cdot \mathbf{B}(x) \right] + \hat{H}_f$$

$$H_f = \mathbb{I} \otimes \mathbb{I} \left(\sum_{q=1}^{N} \sum_{\mu=1}^{3} \frac{e^2}{2} E_{q,\mu}^2 - \sum_{q=1}^{N} \sum_{\mu \neq \nu = 1}^{3} \frac{1}{e^2} W_{q,\mu,\nu}^2 \right)$$

Pauli-Fierz Coulomb Interaction

- Allows interactions to be included using the Coulomb operator.
- Properly treats external fields.
- Useful for laser chemistry experiments

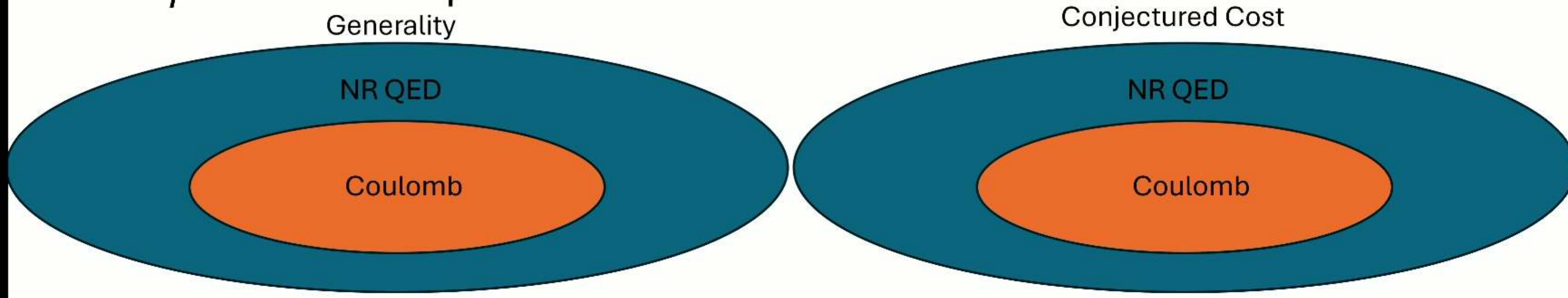


Our Approach to fixing this

- We focus on first quantized simulations because these provide the best asymptotics for Coulomb Hamiltonian.

$$\widetilde{O}(N^{1/3}\eta^{8/3} t \log^2(1/\epsilon))$$

- N = Number of spatial gridpoints,
  η = Number of particles



Approach to fixing this

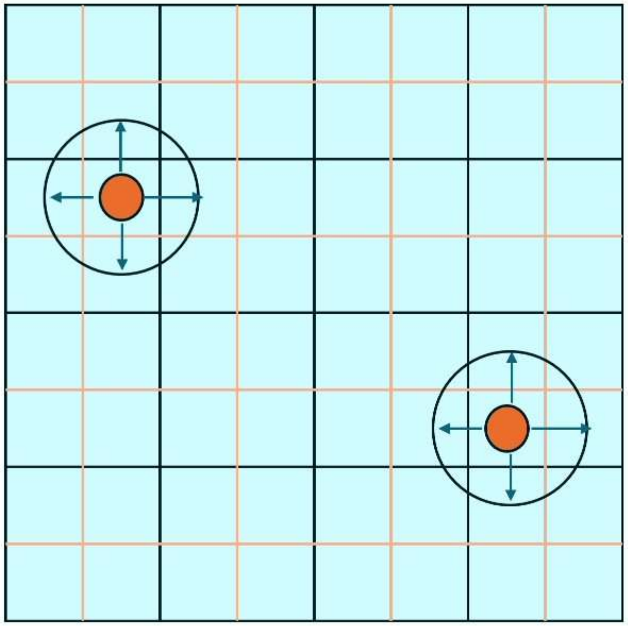
Break the electromagnetic field into M boxes.
(Photons not used because they suck in first quantization)

Build a spatial grid for the particles with N positions.

Place particles on grid sites

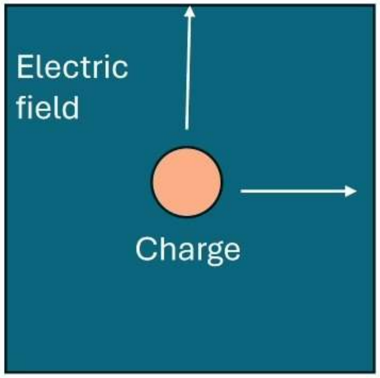
NEW: Impose Gauss' law on particles

These steps are sufficient to build the correct theory.

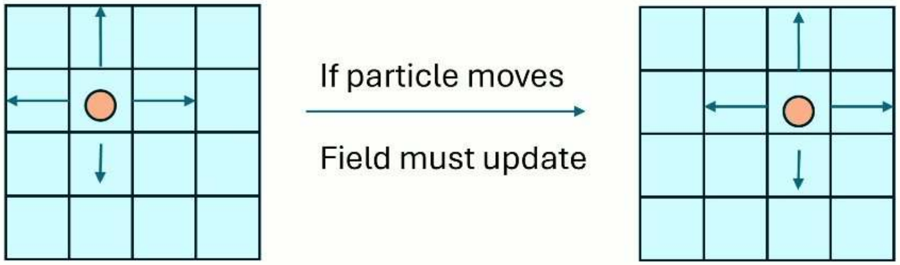


Gauss' Law

$$\oint_S \mathbf{E} \cdot d\mathbf{A} = \frac{Q}{\varepsilon_0}$$



Net electric field flowing out of a box is equal to the charge enclosed in it.
This is one of four essential equations for classical electromagnetism (Maxwell's equations)



Hamiltonian

$$H := H_f + \lambda H_c$$

Hf is the free evolution and Hc is the Gauss' law constraint.
Lambda is a penalty strength that will forbid the dynamics from violating Gauss' law.

$$H_f := \sum_{i=0}^{\eta-1} \frac{1}{2m_i} \sum_{\mu=0}^{2} \left(-i\nabla_{i,\mu} \otimes \mathbb{1} - \zeta_i \sum_{q=0}^{M-1} \mathbb{1} \otimes \delta_{x\in D_q} A_{q,\mu} \right)^2 + \frac{h^3}{8\pi} \sum_{q=0}^{M-1} \sum_{\mu=0}^{2} \mathbb{1} \otimes E_{q,\mu}^2 + \frac{c^2 h^3}{8\pi} \sum_{q=0}^{M-1} \mathbb{1} \otimes |\nabla_q \times A_q|^2$$

Kinetic Energy of Particles

Energy of Electromagnetic Field

Gauss' Law Constraint

Total Charge inside Field Cube

$$H_c = \left(\mathbb{1} - \prod_{q=0}^{M-1} \text{rect} \left(\frac{h^2}{2} \sum_{\mu=0}^{2} \mathbb{1} \otimes \left(E_{q+e_\mu,\mu} - E_{q-e_\mu,\mu} \right) - 4\pi \sum_{i=0}^{\eta-1} \zeta_i \Pi_{q,i} \right) \right)$$

Discrete Approximation to Field Integral

The physically valid states are inside the Kernel of this projector.
It will be helpful later to think of this as a "Code Space"

How Strong Does the Constraint need to be?

Lemma 10 (Lemma 7.1 of Ref. [11]). *Let $H = H_0 + \lambda H_c$ where Hermitian $H_0, H_c \in L(\mathcal{H})$ for $\lambda > 0$ be a variable describing the strength of the constraint such that $\|H_f\|_\infty \ll \lambda$ and $H_c \succeq 0$, such that the dimension of the kernel of H_c is at least 1 and the second smallest eigenvalue is at least 1. We then have that for any $|\psi\rangle$ in the kernel of H_c,*

$$\|e^{-i(H_0+\lambda H_c)t} |\psi\rangle - \lim_{\lambda\to\infty} e^{-i(H_0+\lambda H_c)t} |\psi\rangle \|_2 \leq \epsilon$$

for any $\epsilon > 0$ can be achieved using a choice of the penalty strength that scales a as $\lambda \in \Theta(\|H_0\|_\infty^2 t/\epsilon)$.

- Here we have that the strength of the penalty needs to scale inversely with error.

Hamiltonian

$$H := H_f + \lambda H_c$$

Hf is the free evolution and Hc is the Gauss' law constraint.
Lambda is a penalty strength that will forbid the dynamics from violating Gauss' law.

$$H_f := \sum_{i=0}^{\eta-1} \frac{1}{2m_i} \sum_{\mu=0}^{2} \left(-i\nabla_{i,\mu} \otimes \mathbb{1} - \zeta_i \sum_{q=0}^{M-1} \mathbb{1} \otimes \delta_{x\in D_q} A_{q,\mu} \right)^2 + \frac{h^3}{8\pi} \sum_{q=0}^{M-1} \sum_{\mu=0}^{2} \mathbb{1} \otimes E_{q,\mu}^2 + \frac{c^2 h^3}{8\pi} \sum_{q=0}^{M-1} \mathbb{1} \otimes |\nabla_q \times A_q|^2$$

Kinetic Energy of Particles

Energy of Electromagnetic Field

Solution to problem

- You transform into the interaction frame of the constraint and the electric field.
- This leads to a rapidly varying Hamiltonian, but the coefficients of the Hamiltonian are small.

Definition 9 (Interaction Hamiltonian for Constrained Pauli-Fierz)**.** *Under the assumptions of Definition 8 we define the interaction picture version of the Hamiltonian in the frame of the constraint Hamiltonian and the Electric term to be $H_{\text{int}} : \mathbb{R} \mapsto L(\mathcal{H})$ via*

$$H_{\text{int}}(t) = \sum_{i=0}^{\eta-1} \frac{1}{2m_i} \sum_{\mu=0}^{2} e^{i(\lambda H_c + \frac{h^3}{8\pi} \sum_{q,\mu} \mathbb{1} \otimes E_{q,\mu}^2)t} \left(-i\nabla_{i,\mu} \otimes \mathbb{1} - \zeta_i \sum_{q=0}^{M-1} \mathbb{1} \otimes \delta_{x \in D_q} A_{q,\mu} \right)^2 e^{-i(\lambda H_c + \frac{h^3}{8\pi} \sum_{q,\mu} \mathbb{1} \otimes E_{q,\mu}^2)t}$$
$$+ \frac{c^2 h^3}{8\pi} \sum_{q=0}^{M-1} \sum_{\mu=0}^{2} e^{i(\lambda H_c + \frac{h^3}{8\pi} \sum_{q,\mu} \mathbb{1} \otimes E_{q,\mu}^2)t} \left(|\nabla_\mu \times A_\mu|^2 \right) e^{-i(\lambda H_c + \frac{h^3}{8\pi} \sum_{q,\mu} \mathbb{1} \otimes E_{q,\mu}^2)t}$$

Idea

$$H_c = \left(\mathbb{1} - \prod_{q=0}^{M-1} \mathrm{rect}\left(\frac{h^2}{2} \sum_{\mu=0}^{2} \mathbb{1} \otimes (E_{q+e_\mu,\mu} - E_{q-e_\mu,\mu}) - 4\pi \sum_{i=0}^{\eta-1} \zeta_i \Pi_{q,i} \right)\right)$$

- Naïve algorithm: For each of the M field sites look at each particle and decide whether the particle is in the box (recall they are on different grids).
- Cost: $\tilde{O}(\eta M)$
- Improved: Use merge sort to sort the particles by their positions in the grid.
  Then combine particles into fake particles at center of cell with total charge $\sum_i Q_i$.
  Compute divergence and compare with each charge.

Total Cost of Simulation

- For c = speed of light, Delta = grid spacing, b and a parameters for finite difference formulas used in discretization number of T gates:

$$\widetilde{O}\left(\eta t\left(\frac{Mc^2}{\eta}+\frac{1}{\Delta^2}\right)\left(M(b^3+a^2)+\sum_i|\zeta_i|\right)\log^2(N\Lambda)\log^2(1/\epsilon)\right)$$

- Thermodynamic:

$$\mathcal{C}_{\text{Therm.,QED}}\in\widetilde{O}\left(N^{2/3}\eta^{4/3}t\log^5(1/\epsilon)\right).$$

- Coulomb Potential:

$$\mathcal{C}_{\text{Therm.,Coulomb}}\in\widetilde{O}\left(N^{1/3}\eta^{8/3}t\log^2(1/\epsilon)\right).$$

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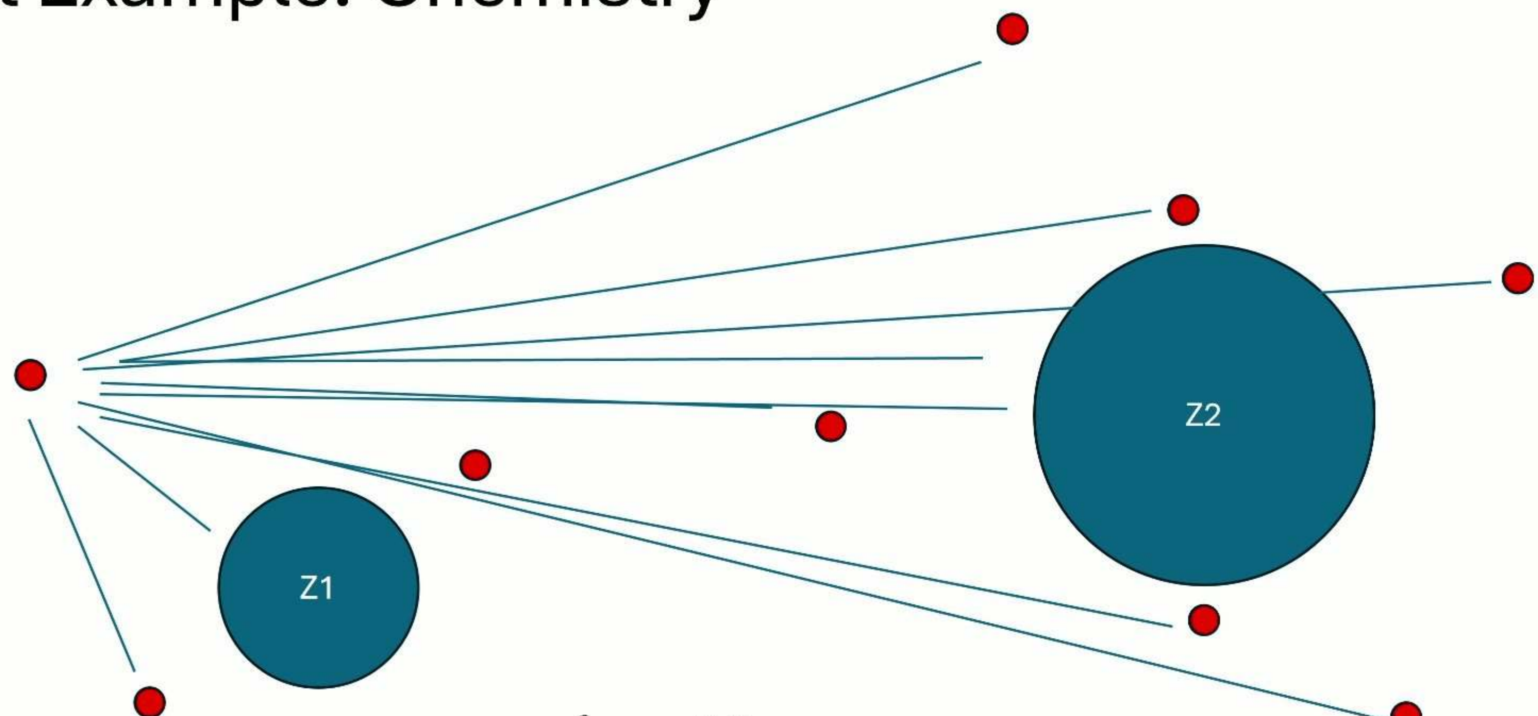

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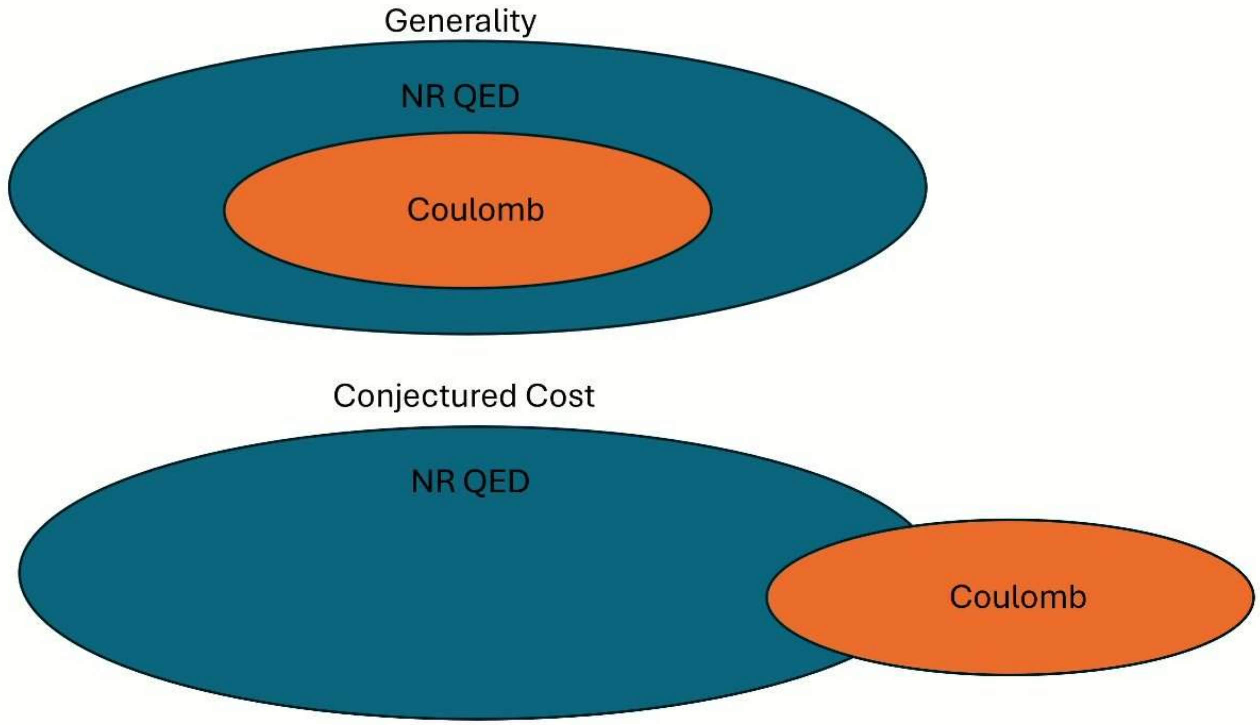
Coulomb can actually be more expensive!



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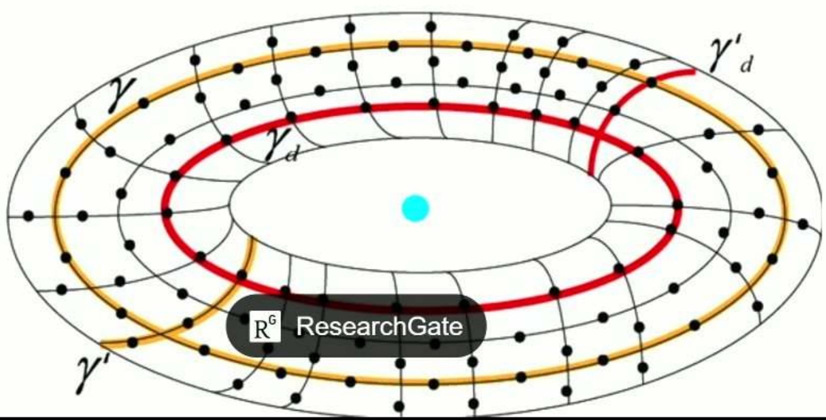
Emergence of Coulomb Interaction

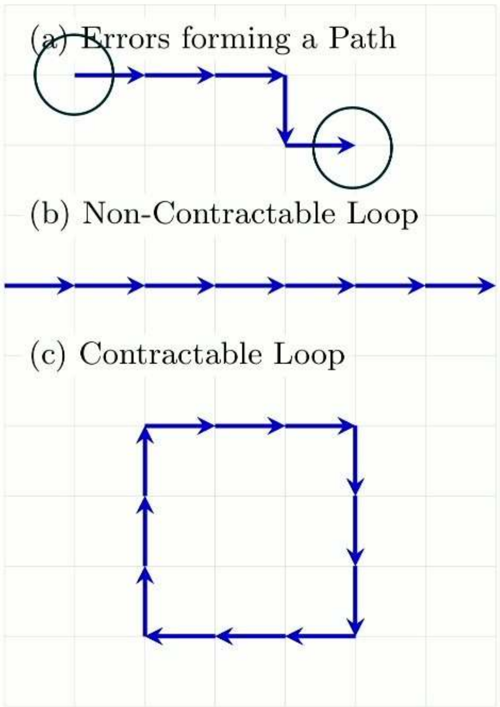
- The emergence of the Coulomb potential though occurs for surprising reasons.
- It emerges because of topological protection in the thermodynamic and nonrelativistic limits.

Toric Code



A tale of three errors

- Consider a background field in the codespace of the Gauss' law projector.
- Imagine we have an error of the form of (a)
- Gauss' law will be violated at end points, this cannot emerge.
- (b,c) correspond to logical errors.



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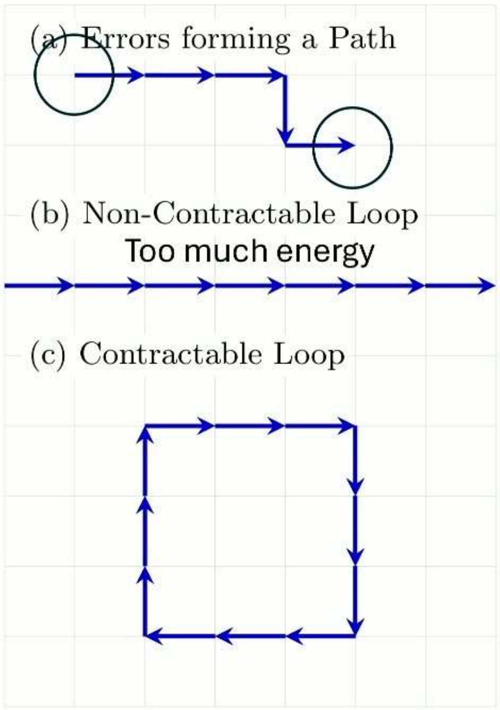
- Imagine we have an error of the form of (a)
- Gauss' law will be violated at end points, this cannot emerge.
- (b,c) correspond to logical errors.
- For (b) The energy of the error scales as $\sum_i E_i^2 \to \infty$ in thermodynamic limit.
- Case (c) cannot occur because of maxwell Faraday in the limit of large c such a loop leads to a large B derivative.



Conclusion

- We started out on this quest to see how much more expensive simulations of chemistry would be if we included electrodynamics.
- We found they were cheaper in some cases because fields simplified the interaction evaluation.
- Further, Coulomb's law can be seen to emerge from topological properties of the simulation (similar to toric code).