# Q-Sim: Perceiving nature through Quantum

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# Today we will discuss...

# Introduction (1)

**What is quantum simulation?**

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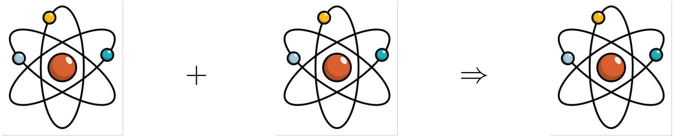
For a particular model of a quantum system, its simulation consists of the ability to **emulate** how the system changes over time.

# Introduction (2)



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The Hamiltonian allows for **time independent Schrödinger's equation**!

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Thus, the **eigenvalues** are $\{E_1, \ldots, E_n\}$.

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**Ground state energy:** $-\hbar\omega$

# Functions applied on diagonal matrices

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$$D = \sum_{k=0}^{n} d_k |k\rangle\langle k| \Rightarrow e^D = \sum_{k=0}^{n} e^{d_k} |k\rangle\langle k|$$

# Schrödinger's equation (1)

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$$\boxed{|\Psi(t)\rangle = \exp\left(-\frac{iHt}{\hbar}\right) \cdot |\Psi(0)\rangle}$$

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So, by differentiation:

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Substituting in **Schrödinger's equation**, we get:

$$i\hbar\frac{d|\Psi\rangle}{dt} = H|\Psi\rangle \Leftrightarrow H|\Psi\rangle = H|\Psi\rangle$$

# Schrödinger's equation (2)

The formula can be rewritten for $t_1$ and $t_2$ instead:

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Trivial proof: $UU^T = \exp\left(-\frac{iH\Delta t}{\hbar}\right) \exp\left(+\frac{iH\Delta t}{\hbar}\right) = I_n$

# More matrix exponentiation

**Please note that:**

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In our case, $H$ and $-H$ do in fact commute.

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$$K = -i \sum_{k=1}^{n} (\log u_k) |k\rangle\langle k|$$

Consider $u_k = e^{i\varphi_k}$, since these are the **eigenvalues of an unitary matrix**:

$$K = \sum_{k=1}^{n} \varphi_k |k\rangle\langle k| \Rightarrow K \text{ is Hermitian}$$

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In order to write the Hamiltonian for a particle moving in space, we need to use the **position basis**.

We define the state of a particle as a function of its position:

$$\langle x|\Psi\rangle = \Psi(x)$$

# Simulating Hamiltonians Classically (2)

$$i\hbar\frac{\partial}{\partial t}\Psi(x) = \left[-\frac{1}{2m}\cdot\frac{\partial^2}{\partial x^2} + V(x)\right]\Psi(x)$$

...where:

1. $-\frac{1}{2m}\cdot\frac{\partial^2}{\partial x^2}$ – kinetic energy part;
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1. $-\frac{1}{2m}\cdot\frac{\partial^2}{\partial x^2}$ – kinetic energy part;
2. $V(x)$ – potential energy part.

In total, $\left[-\frac{1}{2m}\cdot\frac{\partial^2}{\partial x^2} + V(x)\right]$ is the **Hamiltonian** in position basis for some physical particles.

# Simulating Hamiltonians Classically (3)

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- For 2 qubits, we need to solve 4 equations;
- For $k$ qubits, we need to solve $2^k$ equations.

# Local interactions

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This assumes **local interactions**.

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$$H = \sum_{k=1}^{l} H_k$$

Now, $H_k$ is **easy** to approximate. **BUT**, unfortunately, no commutation:

$$e^{-i\sum_k H_k t} \neq \prod_{k=1}^{n} e^{-iH_k t}$$

# Trotter's formula

**Trotter's formula** comes to the rescue:

$$\boxed{\lim_{n\to+\infty}\left[\exp\left(\frac{iAt}{n}\right)\cdot\exp\left(\frac{iBt}{n}\right)\right]^{n} = \exp\left(i(A+B)t\right)}$$

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Or even better:

$$\boxed{\exp(i(A+B)\Delta t) = \exp\left(\frac{iA\Delta t}{2}\right)\cdot\exp(iB\Delta t)\cdot\exp\left(\frac{iA\Delta t}{2}\right) + O(\Delta t^3)}$$

# Schrödinger's equation revised (1)

We have already arrived at the following form:

$$i\hbar \frac{\partial}{\partial t}\Psi(x) = \left[ -\frac{1}{2m} \cdot \frac{\partial^2}{\partial x^2} + V(x) \right] \Psi(x)$$

# Schrödinger's equation revised (1)

We have already arrived at the following form:

$$i\hbar\frac{\partial}{\partial t}\Psi(x) = \left[-\frac{1}{2m}\cdot\frac{\partial^2}{\partial x^2} + V(x)\right]\Psi(x)$$

This means that $H$ can be simply written as:

$$H = -\frac{1}{2m}\cdot\frac{\partial^2}{\partial x^2} + V(x) = \boxed{\frac{p^2}{2m} + V(x)}$$

# Schrödinger's equation revised (2)

At the same time, the wave function can be written as:

$$|\Psi\rangle = \int_{-\infty}^{\infty} |x\rangle\langle x|\Psi\rangle \, dx$$

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In total, there are $\frac{2d}{\Delta x} + 1$ chunks – but the chunk can express $2^n$ equations!

# Schrödinger's equation revised (3)

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**Conclusion:** In practice, using qubits instead of classical bits reduces the complexity from $O(2^n)$ to $O(n^2)$!

# Conclusion (1)

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This whole presentation described Hamiltonians, which are at the heart of **quantum chemistry simulations**!

# Conclusion (2)

Consider the following molecular Hamiltonian:

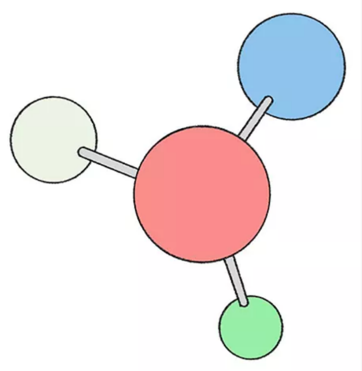
$$H = EKE + NKE + ENC + EEC + NNC$$

Where:

1. $EKE = -\sum_{i=1}^{M} \frac{1}{2}\nabla_i^2$, the electron kinetic energy;
2. $NKE = -\sum_{A=1}^{M} \frac{1}{2MA}\nabla_A^2$, the nucleus kinetic energy;
3. $ENC = -\sum_{i=1}^{N} \sum_{i=1}^{M} \frac{Z_A}{r_iA}\nabla_A^2$, the electron-nucleus coulomb energy;
4. $EEC = \sum_{j>i} \frac{1}{r_{ij}}$, the electron-electron coulomb energy;
5. $NNC = \sum_{B>A} \frac{Z_A Z_B}{r_{AB}}$, the nucleus-nucleus coulomb energy;

# Conclusion (3)

Using that formula, alongside **Born-Oppenheimer's approximation** *(nuclei are fixed in space)*, molecules can be **modeled!**



# References

For this presentation, I recommend:

- *Quantum Computation and Quantum Information* (Nielsen, Chuang)
    - 2.2.2. Evolution;
    - 4.7. Simulation of quantum systems.
- Qiskit's 2022 summer school materials;
- Qiskit's 2020 summer school materials.

# The end

Thank you!

This presentation was held for the IQC course.