Hamiltonian Simulation Theory

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The theory of computation taught us that the details of the computational model – whether it's a Turing Machine, python code, Conway's game of life – matter less than <u>what</u> is being computed. The way the computation manifests might look very different in these different models – TM transition rules updating symbols on a linear tape, if/for/while statements, live & dead cells propagating and dying. But the way the <u>information</u> encoded in the system is being processed is the same. If we understand the computation in one model, we understand it in any other model.

Moreover, there are universal models of computation: simple specific instances that are able to replicate <u>any</u> computation that that, or any other, model of computation can compute. E.g. a universal Turing Machine.

Analogously, in physics, two completely different physical systems can turn out to be entirely equivalent, such that understanding the behaviour of one system means we also understand the behaviour of the other. A classic example from undergraduate physics is mechanical systems of linked masses and springs, and LCR circuits in electronics.

When are two physical systems equivalent in this way?

Understanding this equivalence in general, or even just particular instances of it, has fruitful applications all over physics, from electromagnetism, to computing the critical point of the classical Ising model (via the Kramers-Wannier duality), to strong/weak dualities in quantum field theory that allow perturbative methods to be applied to strongly interacting systems, to holographic dualities in quantum gravity, to using cold atom arrays to simulate high-T_c solid state superconductors in analogue Hamiltonian simulation.

In this course, we will build up a rigorous mathematical theory of Hamiltonian simulation, which gives one answer to the above question of when two systems are physically equivalent. And this formalism will turn out to be very fruitful, leading to the discovery of universal many-body models that contain all possible many-body physics, analogous to universal Turing Machines in computation theory. To a full complexity classification of all 2-qubit interactions in Hamiltonian complexity. Even to applications in quantum gravity (beyond the scope of this lecture series, but see Tamara's course).

(Very incomplete) History & References

Hamiltonian Complexity:

[Barahona '82]
Proved NP-completeness of ground state energy problem for classical Ising model with fields, connecting computational complexity theory with physics (stat. mech.)

[Kitaev ~'02]
QMA-completeness of quantum ground state energy problem ("local Hamiltonian problem"), for k-local Hamiltonians with $k = 5$.

[KKR '04]
Introduced "perturbation gadgets" technique, to prove QMA-completeness for $k = 2$.

[OT '08]
Extended perturbation gagets to a general framework, to prove QMA-completeness for nearest-neighbour qubit Hamiltonians on a lattice.

[BDL '11]
Developed alternative perturbation gadget analysis via Schrieffer-Wolff perturbation theory formalism.

[CM '16]
Proved quantum generalisation of Shaeffer's dichotomy Thm. giving complete classification of complexity of 2-local qubit Hamiltonians.

[BH '17]
Pinned down complexity of quantum transverse Ising model (3rd class in [CM '16] classification Thm.), thereby completing the classification, making use of Schrieffer-Wolff formalism

<u>"Complete Hamiltonians"</u>:

[de las Cuevas, Dür, Briegel et al. '08]
Proved that partition functions $Z_H(\beta) = \sum_{\sigma} e^{-\beta H(\sigma)}$ of certain classical Hamiltonians are "complete", i.e. can reproduce the partition function of <u>any</u> other classical Hamiltonian.

[dLCC'16]

Proved that there exist "universal classical Hamiltonians", which can exactly reproduce all physics of any other classical Hamiltonian. Proved that H is universal iff its ground state energy problem is NP-complete.

Quantum Hamiltonian simulation:

[CMP'19]

Developed mathematical framework of (analogue) quantum Hamiltonian simulation. Proved that there exist universal quantum Hamiltonians, which can reproduce all physics of any other Hamiltonian to arbitrarily high accuracy. Proved complete classification of simulation power of 2-local qubit Hamiltonians.

When does one Hamiltonian H' simulate another H ?

Mathematics teaches us it's often fruitful to study the maps between objects, rather than the objects themselves.

Can rephrase this as:

What are the maps

$$\mathcal{E}: \mathrm{Herm} \to \mathrm{Herm}$$
$$H \longrightarrow H' = \mathcal{E}(H)$$

which preserve all the physics of H ?

What does it mean to "preserve all the physics" ?

Information theory teaches us that it's fruitful to take an operational approach. So let's list everything that's accessible in principle in experiment, and ask that the map $\mathcal{E}$ preserves it all.

Notation

$\mathcal{B}(\mathcal{H})$: set (actually, algebra) of all bounded operators on Hilbert space $\mathcal{H}$

$\mathcal{M}_n$: $n \times n$ complex matrices

Herm_n : $n \times n$ Hermitian matrices
$H \in \mathrm{Herm}_n \iff H^\dagger = H$

$\mathrm{Herm}(\mathcal{H})$: Hermitian operators on Hilbert space $\mathcal{H}$

$\bar{z}$: complex conjugate of $z \in \mathbb{C}$

$\bar{M}$: entry-wise complex conjugation of $M \in \mathcal{M}_n$.

$[a,b]$: closed interval a to b in $\mathbb{R}$, i.e. $[a,b] = \{x \in \mathbb{R} : a \leq x \leq b\}$

$$M^{\oplus n} := \underbrace{M \oplus M \oplus \cdots \oplus M}_{n \text{ times}}$$

$\mathrm{spec}(M)$: spectrum of M (i.e. set of eigenvalues) <u>not</u> including degeneracies

$\mathbb{1}_d$: d-dimensional identity matrix

$\mathrm{Re}(X)$, $\mathrm{Im}(X)$: real, imag parts of X (entry-wise for $X \in \mathcal{M}_d$)

Hamiltonian Encodings

Hamiltonian $H \in \mathrm{Herm}_n$
Observables $A, B \in \mathrm{Herm}_n$
State $\rho \in \mathrm{Herm}_n$, $\mathrm{tr}\,\rho = 1$

1. $A' = \mathcal{E}(A)$ should be Hermitian
   $\Rightarrow \mathcal{E}$ Hermiticity preserving:
   $\mathcal{E}(A)^\dagger = \mathcal{E}(A)$

2. Eigenvalues of A correspond to measurement outcomes $\Rightarrow \mathcal{E}$ spectrum preserving:
   $\mathrm{spec}(\mathcal{E}(A)) = \mathrm{spec}(A)$

3. Probabilistic combinations of observables correspond to experiments we can perform
   $\Rightarrow \mathcal{E}$ convex:
   $$\mathcal{E}(pA + (1-p)B) = p\,\mathcal{E}(A) + (1-p)\,\mathcal{E}(B)$$

4. Expectation values of observables should be preserved:
   $\mathrm{tr}(A\rho) = \mathrm{tr}(\mathcal{E}(A)\,\mathcal{E}(\rho))$

5. Time-dynamics:
   $$\mathrm{tr}(\mathcal{E}(A)\, e^{-it\mathcal{E}(H)}\, \mathcal{E}(\rho)\, e^{it\mathcal{E}(H)}) = \mathrm{tr}(A\, e^{-itH} \rho\, e^{-itH}).$$

6. Thermodynamic properties
$\Rightarrow$ partition function should be preserved (up to irrelevant rescalings & additive shifts, as these don't affect the physics):

$$Z_{H'} = \mathrm{tr}\left(e^{-\beta \mathcal{E}(H)}\right) = \gamma\, \mathrm{tr}\left(e^{-\beta H}\right) + \alpha.$$

7. Should be able to construct simulation of many-body Hamiltonian $H = \sum_i \alpha_i h_i$ term-by-term, not globally
$\Rightarrow$ $\mathcal{E}$ linear over reals:

$$\forall \alpha_i \in \mathbb{R},\ h_i \in \mathrm{Herm}$$
$$\mathcal{E}\left(\sum_i \alpha_i h_i\right) = \sum_i \alpha_i\, \mathcal{E}(h_i)$$

...

In fact just 1–3 already suffice to ensure all physics is preserved by $\mathcal{E}$!

Thm (encodings)

$\mathcal{E}: \mathrm{Herm}_n \to \mathrm{Herm}_n$

The followin gare equivalent:

(i) $\forall A, B \in \mathrm{Herm}_n$, $\forall p \in [0,1]$

1. $\mathcal{E}(A) = \mathcal{E}(A)^\dagger$
2. $\mathrm{spec}(\mathcal{E}(A)) = \mathrm{spec}(A)$
3. $\mathcal{E}(pA + (1-p)B) = p\,\mathcal{E}(A) + (1-p)\,\mathcal{E}(B)$

(ii) $\exists$ unique extension $\mathcal{E}': \mathcal{M}_n \to \mathcal{M}_m$ s.t. $\mathcal{E}'(H) = \mathcal{E}(H)$ for all $H \in \mathrm{Herm}_n$, & $\forall A, B \in \mathcal{M}_n$, $\forall x \in \mathbb{R}$:

a. $\mathcal{E}'(\mathbb{1}) = \mathbb{1}$

b. $\mathcal{E}'(A^\dagger) = \mathcal{E}'(A)^\dagger$

c. $\mathcal{E}'(A+B) = \mathcal{E}'(A) + \mathcal{E}'(B)$

d. $\mathcal{E}'(AB) = \mathcal{E}'(A)\,\mathcal{E}'(B)$ ← this is the non-trivial one

e. $\mathcal{E}'(xA) = x\,\mathcal{E}'(A)$

(iii) $\exists$ unique extension $\mathcal{E}': \mathcal{M}_n \to \mathcal{M}_m$ s.t. $\mathcal{E}'(H) = \mathcal{E}(H)$ for all $H \in \mathrm{Herm}_n$, with $\mathcal{E}'$ of form

$$\mathcal{E}'(M) = U(M^{\oplus p} \oplus \bar{M}^{\oplus q})\,U^\dagger$$

for some $p, q \geq 0$, unitary $U \in \mathcal{M}_m$.

We call such an $\mathcal{E}$ an <u>encoding</u>.

Note (iii) is basis-independent, despite complex conjugation, as change of basis can be absorbed in U.

<u>Lemma</u>

$\mathcal{E}: \mathrm{Herm}_n \longrightarrow \mathrm{Herm}_n$
Convexity + spectrum preserving
$\Rightarrow$ real linearity

<u>Pf</u>

Spectrum preserving $\Rightarrow \mathcal{E}(0) = 0$.

$\lambda < 0$,
set $p = \frac{\lambda}{\lambda - 1}$

Use 3 $\Rightarrow \mathcal{E}(\lambda A) = \lambda\, \mathcal{E}(A) \quad (*)$

Apply $(*)$ to $\lambda A \Rightarrow \mathcal{E}(\lambda^2 A) = \lambda^2 \mathcal{E}(A)$

$\square$

To prove Thm, we will need to take a brief mathematical detour into Jordan algebras and Jordan rings.

Jordan Rings

Def. (Ring)

Set R, binary operations $\cdot$, $+$

- Abelian group over $+$
- closure: $ab \in R$
- associative: $(ab)c = a(bc)$
- identity: $1 \cdot a = a \cdot 1 = a$

Example: matrices over $\mathbb{C}$ with usual matrix multiplication.

Def. (Special Jordan Ring)

R_J obtained from R by replacing product with symmetric product $a \circ b = ab + ba$.

Not associative! $(a \circ b) \circ c \neq a \circ (b \circ c)$

But is commutative: $a \circ b = b \circ a$.

Why do we care about these weird non-associative structures in quantum mechanics?!

Example

$\mathrm{Herm}_n \subset M_n$ with symmetric product $A \circ B = AB + BA$ forms a Jordan ring.

So Hermitian observables in QM "naturally" form a Jordan algebra.

Indeed, this was the original motivation for the definition & study of Jordan algebras.

Def. (Ring homomorphism)

Rings R, R', $\phi: R \longrightarrow R$

- $\phi(a+b) = \phi(a) + \phi(b)$
- $\phi(ab) = \phi(a)\phi(b)$
- $\phi(1) = 1$

Def. (Ring anti-homomorphism)

Rings R, R', $\phi: R \longrightarrow R$ s.t.

- $\phi(a+b) = \phi(a) + \phi(b)$
- $\phi(ab) = \phi(b)\phi(a)$ note order!
- $\phi(1) = 1$

<u>Def.</u> (Jordan homomorphism)

$\phi : R_J \longrightarrow R_J$ s.t.

- $\phi(a+b) = \phi(a) + \phi(b)$
- $\phi(a \circ b) = \phi(a) \circ \phi(b)$

<u>Lemma</u>

If R is not of characteristic 2 (i.e. $a^2 \neq 0$), ϕ Jordan homomorphism iff

- $\phi(a+b) = \phi(a) + \phi(b)$
- $\phi(a^2) = \phi(a)^2$

<u>Pf</u>

"if":

$$(a+b)\circ(a+b) = 2a\circ b + a^2 + b^2$$

$$\phi((a+b)^2) = \cancel{2}\phi(a\circ b) + \cancel{\phi(a^2)} + \cancel{\phi(b^2)}$$

$$\parallel$$

$$\phi(a+b)^2 = (\phi(a) + \phi(b))^2$$

$$= 2\phi(a)\circ\phi(b) + \phi(a)^2 + \phi(b)^2$$

$$= \cancel{2}\phi(a)\circ\phi(b) + \cancel{\phi(a^2)} + \cancel{\phi(b^2)}$$

"only if": easy.

Thm. (unique extension)

$\forall n \geq 2$ any Jordan hom. of Herm_n can be extended in one and only one way to a hom. of $\mathcal{M}_n$.

Pf.

$n \geq 3$: Jacobson & Rickart '52

$n = 2$: Martindale '67

Lemma

$\phi : \mathrm{Herm}_n \longrightarrow \mathrm{Herm}_m$

- unital : $\phi(\mathbb{1}) = \mathbb{1}$
- invertibility preserving:
  H invertible $\Rightarrow$ $\phi(H)$ invertible
- real linear : $\forall \lambda, \mu \in \mathbb{R}$, $A, B \in \mathrm{Herm}_n$
  $\phi(\lambda A + \mu B) = \lambda \phi(A) + \mu \phi(B)$

ϕ is Jordan hom.

Pf.

$\phi(H - \lambda \mathbb{1}) = \phi(H) - \lambda \mathbb{1}$

+ invertibility-preserving

$\Rightarrow$ $\mathrm{spec}(\phi(H)) = \mathrm{spec}(H)$

$\Rightarrow$ $\forall$ projector P

$\mathrm{spec}(\phi(P)) \in \{0, 1\}$

$+ \ \phi(P)$ Hermitian

$\Rightarrow \ \phi(P)$ projector

$H \in \mathrm{Herm}_n$

spectral decomposition:

$$H = \sum_i \lambda_i P_i$$

$\lambda_i \in \mathbb{R}$, $\quad P_i$ mutually orthog. projectors.

$\forall \ i \neq j : \quad P_i + P_j$ projector

$\Rightarrow \phi(P_i + P_j)$ projector

$$(\phi(P_i + P_j))^2 = \phi(P_i + P_j) = \cancel{\phi(P_i)} + \cancel{\phi(P_j)}$$

$$\shortparallel$$

$$\begin{aligned}(\phi(P_i) + \phi(P_j))^2 &= \phi(P_i)^2 + \phi(P_j)^2 \\ &\quad + \phi(P_i)\phi(P_j) + \phi(P_j)\phi(P_i) \\ &= \cancel{\phi(P_i)} + \cancel{\phi(P_j)} \\ &\quad + \phi(P_i)\phi(P_j) + \phi(P_j)\phi(P_i)\end{aligned}$$

$$\Rightarrow \quad \phi(P_i)\phi(P_j) + \phi(P_j)\phi(P_i) = 0$$

$$\begin{aligned}\phi(H)^2 &= \sum_i \lambda_i^2 \phi(P_i)^2 + \overbrace{\cancel{\sum_{i \neq j} \lambda_i \lambda_j \phi(P_i)\phi(P_j)}}^{=0} \\ &= \sum_i \lambda_i^2 \phi(P_i) \\ &= \phi(H^2) \qquad \square\end{aligned}$$

Back to ...

Pf. (of encodings Thm.)

(i) $\Rightarrow$ (ii):

Unital + invertability preserving (2)
+ real linear (Lemma)
$\Rightarrow$ $\mathcal{E}$ Jordan hom.

Unique extension Thm:
$\exists$ $\mathcal{E}' : \mathcal{M}_n \longrightarrow \mathcal{M}_n$ ring hom.
$\Rightarrow$ $\mathcal{E}'(AB) = \mathcal{E}'(A)\,\mathcal{E}'(B)$. $\Rightarrow$ d.

a, b, c, e: Exercise

(ii) $\Rightarrow$ (iii):
(Write $\mathcal{E} \equiv \mathcal{E}'$ here for brevity)

$J := \mathcal{E}(i\mathbb{1}) \equiv \mathcal{E}(i)$
$J^2 = \mathcal{E}(i)\,\mathcal{E}(i) = \mathcal{E}(i^2) = \mathcal{E}(-1) = -\mathbb{1}$
"complex structure"
$\Rightarrow$ eigvals $J = \pm 1$

$$
\begin{aligned}
J\,\mathcal{E}(A) &= \mathcal{E}(i)\,\mathcal{E}(A) = \mathcal{E}(iA) \\
&= \mathcal{E}(Ai) = \mathcal{E}(A)\,\mathcal{E}(i) \\
&= \mathcal{E}(A)\,J
\end{aligned}
$$

$\Rightarrow$ $\forall A$: $J, \mathcal{E}(A)$ simultaneously diag.

Decompose $A = A_+ \oplus A_-$ acting on on ± 1 eigenspaces of J resp.

$$\mathcal{E}(A)|_\pm = A_\pm$$

$$\mathcal{E}(iA)|_\pm = \pm i\, A_\pm$$

$$\mathcal{E}(AB)|_\pm = A_\pm\, B_\pm$$

$$\mathcal{E}(A^\dagger)|_\pm = A_\pm^\dagger$$

$\Rightarrow$ $\mathcal{E} = \mathcal{E}_+ \oplus \mathcal{E}_-$ is direct sum of

$\mathcal{E}_+(A) := \mathcal{E}(A)|_+$ $*$-representation

$\mathcal{E}_-(A) := \mathcal{E}(A)|_-$ anti-$*$-representation

of C^* algebra $(\mathcal{M}_n, \dagger)$

<u>Lem.</u> (e.g. [Davidson] book)
Any $*$-rep. of finite-dim. C^* alg is unitarily equiv. to direct sum of identity representations.

<u>Cor</u>
Any anti-$*$-rep is direct sum of complex conjugates of identity reps.

$$\Rightarrow \mathcal{E}(A) = \mathcal{E}_+(A) \oplus \mathcal{E}_-(A)$$
$$= U\,(A^{\oplus p} \oplus \bar{A}^{\oplus q})\,U^\dagger$$

(iii) $\Rightarrow$ (i): easy (direct verification) $\square$

Example (Complex-to-real)

$\varphi : \mathcal{B}(\mathbb{C}^d) \longrightarrow \mathcal{B}(\mathbb{R}^{2d})$

$\varphi(M) = \mathrm{Re}(M) \oplus \mathrm{Re}(M) + J\, \mathrm{Im}(M) \oplus \mathrm{Im}(M)$

where $J := iY \otimes \mathbb{1}_d$

$\varphi(M) = U(M \oplus \bar{M})U^\dagger$

where $U = \frac{1}{\sqrt{2}} \begin{pmatrix} \mathbb{1} & \mathbb{1} \\ i\mathbb{1} & -i\mathbb{1} \end{pmatrix}$

$\Rightarrow$ φ is an encoding by Thm. (iii).

Exercise:

Prove that encoding preserves all physics: expectation values, time-dynamics, partition function, etc.

Note: for this, you will need to define an associated map $\mathcal{E}_{state}$ on states related to a given encoding $\mathcal{E}$.

For the purposes of this course, take this to be:

$$\mathcal{E}_{state}(\rho) = U(\rho \oplus 0^{p+q-1})U^\dagger .$$

and assume that $p \geq 1$.