Energy localization, quantum chaos, and the melt-down of digital quantum simulation

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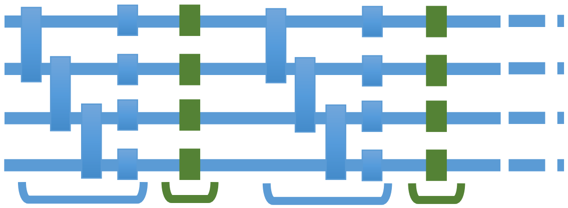
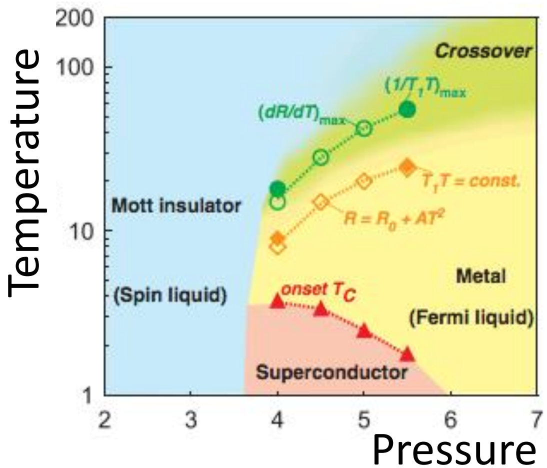
Trieste, 13.9.2017



Digital quantum simulation could solve important physics problems

Condensed matter
(high-T_c superconductivity)



High-energy
(QCD...)

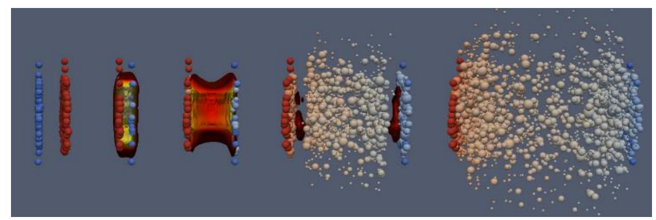
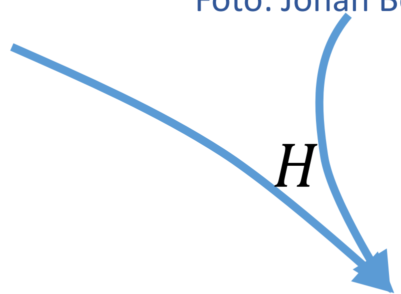


Foto: Jonah Bernhard



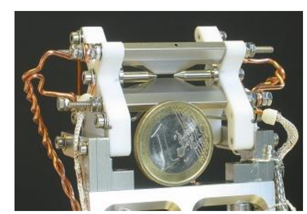
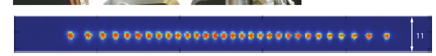
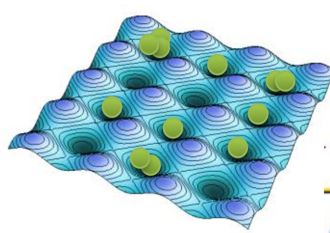


Foto:
Blatt
group





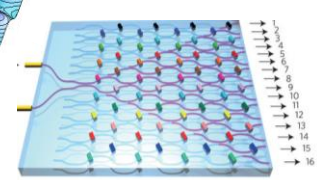


Foto: Crespi et al.,
Nat. Photon 2013

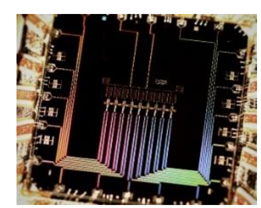


Foto:
Julian
Kelly,
Martinis
group

Digital quantum simulation approximates time evolution operator by discrete gates

Want

$$H = \sum_{l=1}^{M} H_l$$

$$U(t) = \exp[-itH]$$

$$\approx$$

Can do

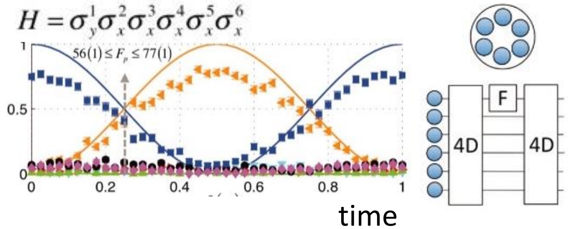
$$H_l \ , \quad U_l(t) = \exp[-itH_l]$$

$$U^{(n)}(t) = \left[U_1\left(\frac{t}{n}\right) U_2\left(\frac{t}{n}\right) \cdots U_M\left(\frac{t}{n}\right)\right]^n$$

Lloyd, Science 1996; Trotter, Proc. Am. Math. Soc. 1959; Suzuki, Prog. Theor. Phys. 1976

Proof-of-principle experiments exist for digital quantum simulation

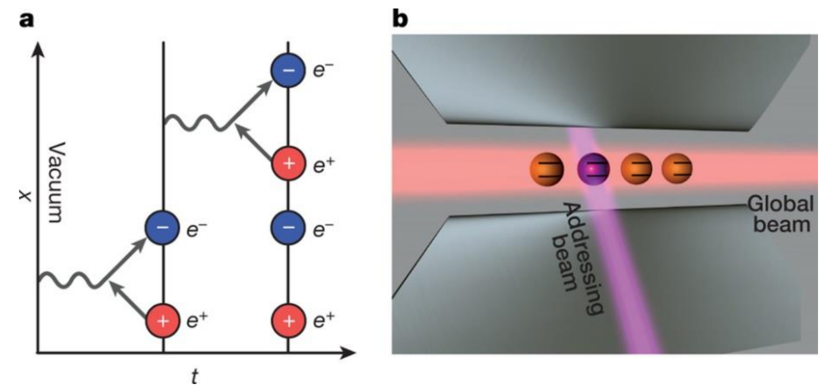
Dynamics of spin models

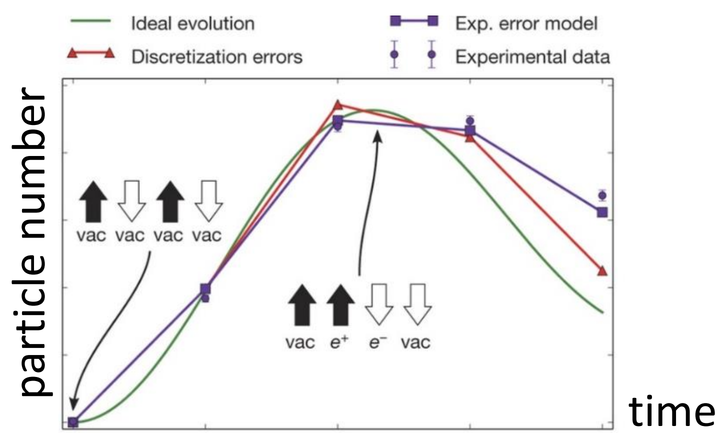


Lanyon et al., Science 2011

See also Salathé et al., PRX 2015

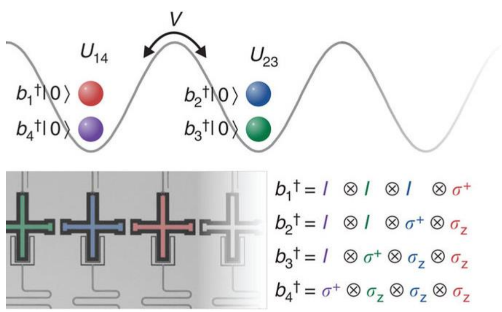
Toy-model lattice gauge theory





Martinez, Muschik, Schindler, Nigg, Erhard, Heyl, PH, Dalmonte, Monz, Zoller, and Blatt, Nature 2016

Fermionic models



Barends et al., Nat. Comm. 2015

How reliable/scalable is that?

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Trotterization has a well-controlled error bound

$$U(t) = \exp[-itH] \quad \approx \quad U^{(n)}(t) = \left[U_1\left(\frac{t}{n}\right) U_2\left(\frac{t}{n}\right) \cdots U_M\left(\frac{t}{n}\right) \right]^n$$

$$U(t) - U^{(n)}(t) = \frac{t^2}{2n} \sum_{l>m=1}^{M} [H_l, H_m] + \mathcal{O}\left(\frac{t^3}{n^2}\right)$$

Polynomial divergence in t and N (# of qubits)

Lloyd, Science 1996

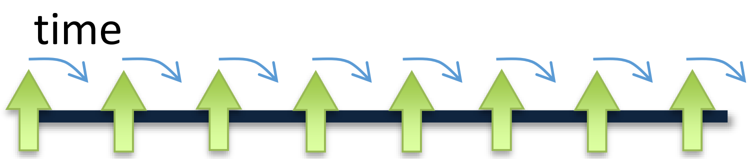
See also
Aharonov and Ta-Shma, in Proc. 35th STOC
Berry, Ahokas, Cleve, and Sanders, Commun. Math. Phys. 2007
Brown, Munro, and Kendon, Entropy 2010
Childs and Kothari, Lecture Notes in Computer Science 2011

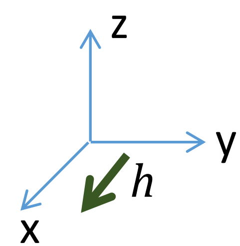
That is a worst case estimate

But maybe for our interests
that is too much!

Local observables may be much more robust than the total unitary

Toy model: trivial time evolution





$$H = h \sum_i \sigma_i^x$$

If the field is modified, unitary changes very fast

$$H = h\sum_i \sigma_i^x \qquad U_h(t) = \bigotimes_i (\cos(ht) - i\sin(ht)\sigma_i^x)$$
$$U_{\tilde{h}}(t) = \bigotimes_i (\cos(\tilde{h}t) - i\sin(\tilde{h}t)\sigma_i^x)$$

Error in unitary

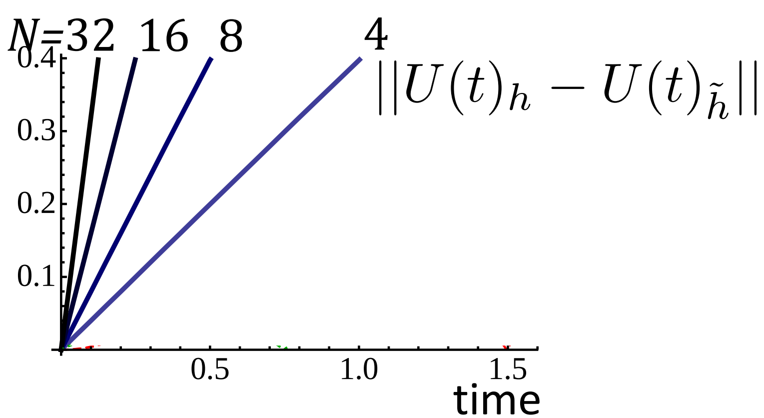
$$U_h(t) - U_{\tilde{h}}(t) =$$
$$iN(\tilde{h} - h)t\sigma_i^x + \mathcal{O}(t^2)$$

Only short times
and small systems!

Error in magnetization

$$\frac{1}{N}\sum_i \langle\sigma_i^z(t)\rangle_h - \frac{1}{N}\sum_i \langle\sigma_i^z(t)\rangle_{\tilde{h}}$$

Independent of N !



What about
digital quantum simulation and
quantum many-body systems?

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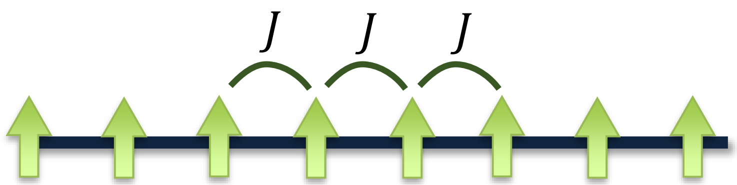
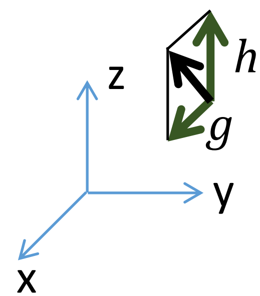
Numerical example:
Ising chain in transverse and longitudinal field

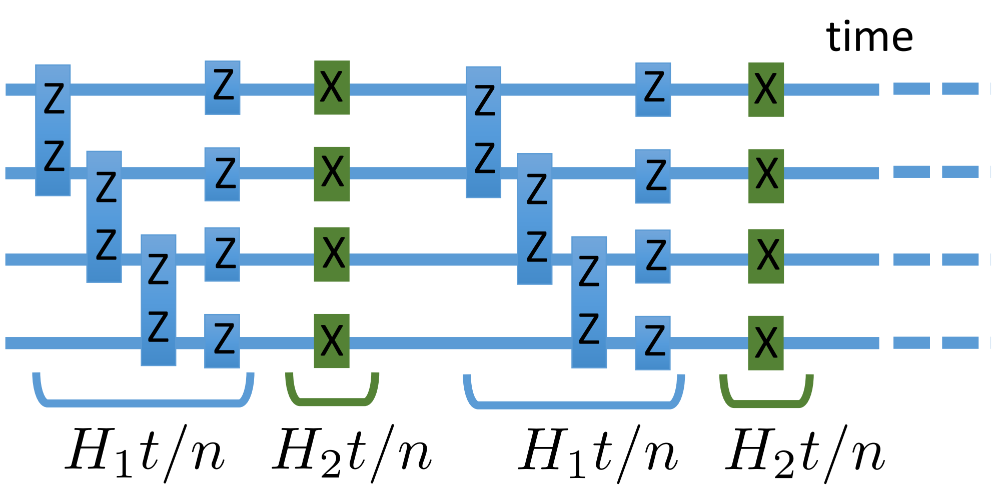




$$H = H_1 + H_2$$

$$H_1 = J\sum \sigma_i^z \sigma_{i+1}^z + h\sum \sigma_i^z$$

$$H_2 = g\sum \sigma_i^x$$



Characterization through energy as an emergent constant of motion

In Trotterized evolution: $E_\tau(t) = \langle\psi_0|\, U_\tau^\dagger(t)\, H\, U_\tau(t)\, |\psi_0\rangle$

$$U_\tau(t) = U^{(n)}(t) = \left[U_1\left(\frac{t}{n} = \tau\right) \ldots U_M\left(\frac{t}{n} = \tau\right)\right]^n$$

Ideally: $E_{\tau=0}(t) = \langle\psi_0|\, e^{i\,H\,t} H e^{-\,i\,H\,t} |\psi_0\rangle = \mathrm{const}$

Simulator fidelity:

$$Q(t) = \frac{E_\tau(t) - E_{\tau=0}}{E_{T=\infty} - E_{\tau=0}}$$

Heating above ideal evolution

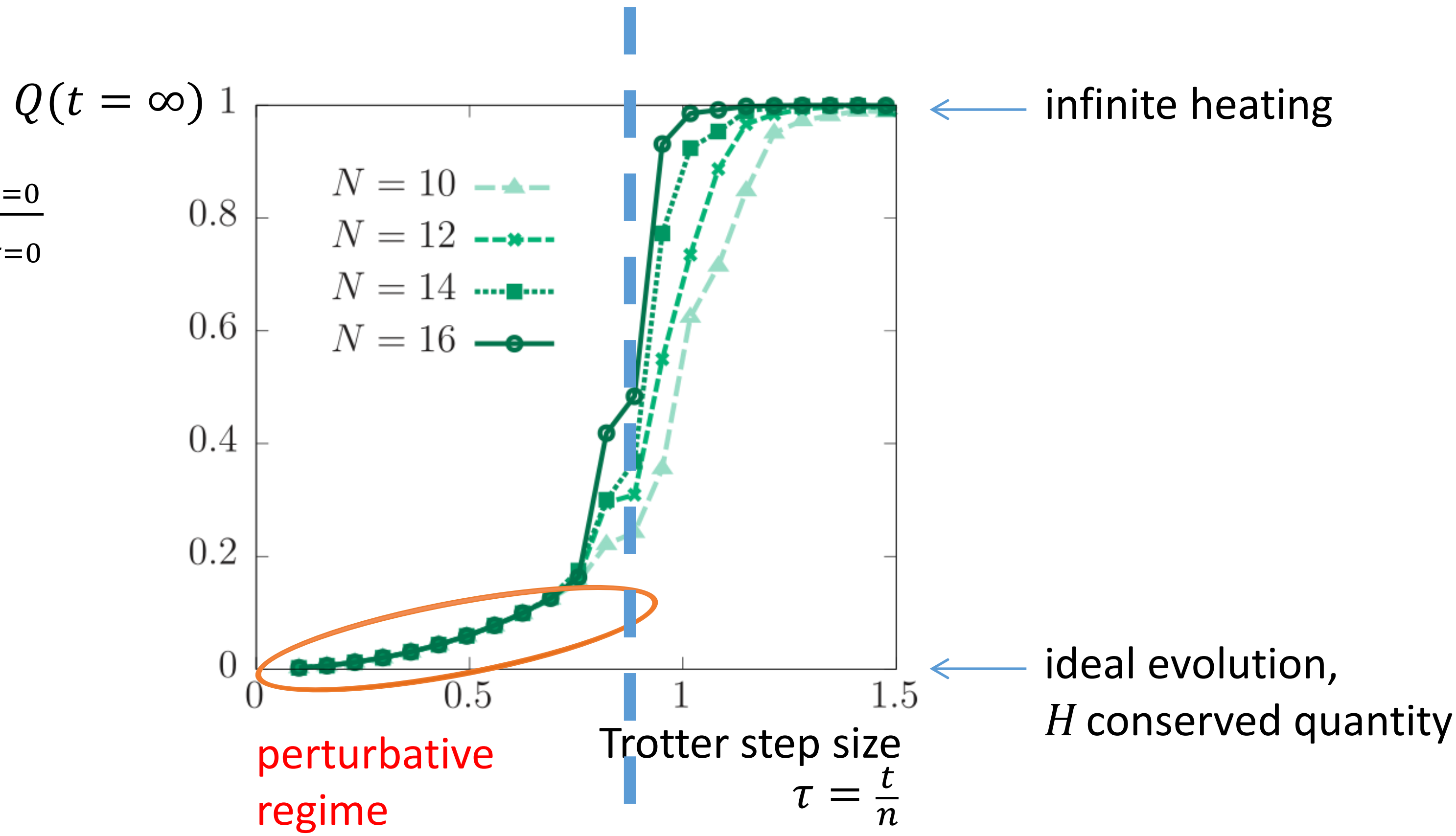
Ideally: $Q = 0$

Normalized to infinite heating

Worst case: $Q = 1$

At small Trotter step, local observables become robust

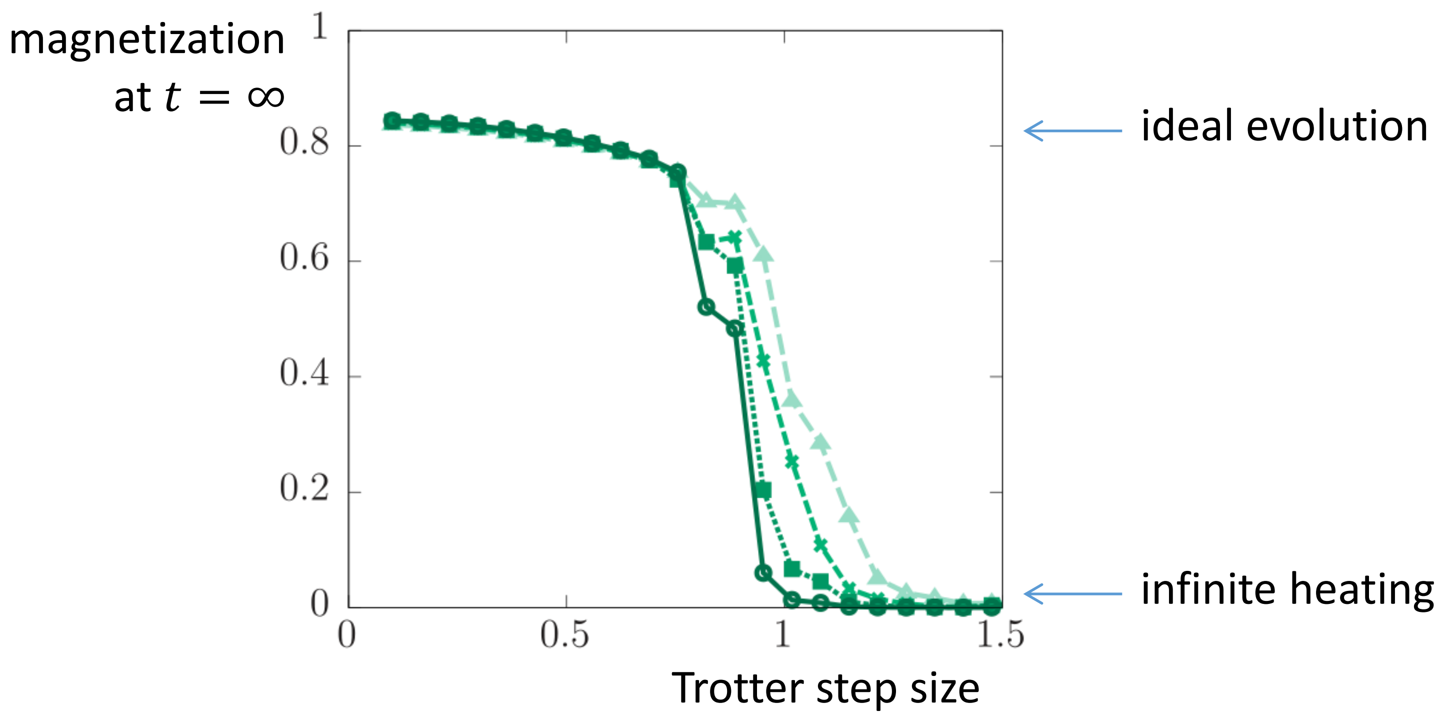
$$Q(t) = \frac{E_\tau(t) - E_{\tau=0}}{E_{T=\infty} - E_{\tau=0}}$$



Compare Lloyds bound

$$U(t) - U^{(n)}(t) = \frac{t^2}{2n} \sum_{l>m=1}^{M} [H_l, H_m] + \mathcal{O}\left(\frac{t^3}{n^2}\right)$$

Not only the energy, also other local observables become robust



Where does that come from?

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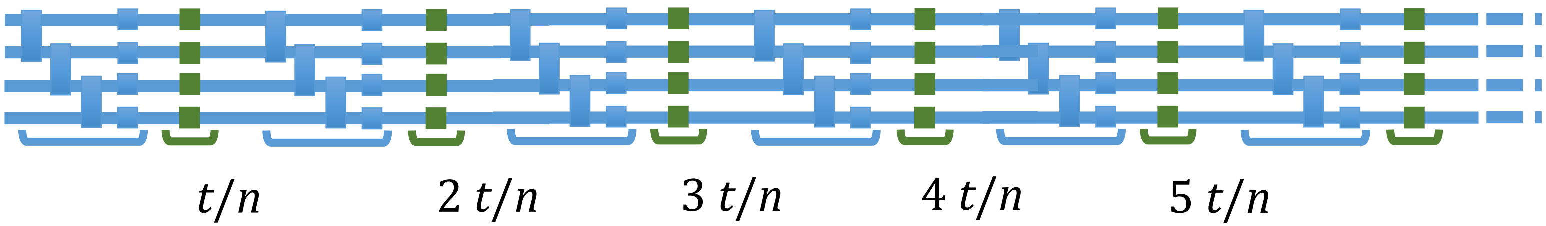
Interpret Trotter sequence as periodic driving

$$U^{(n)}(t) = \left[U_1\left(\frac{t}{n}\right) U_2\left(\frac{t}{n}\right) \cdots U_M\left(\frac{t}{n}\right) \right]^n$$



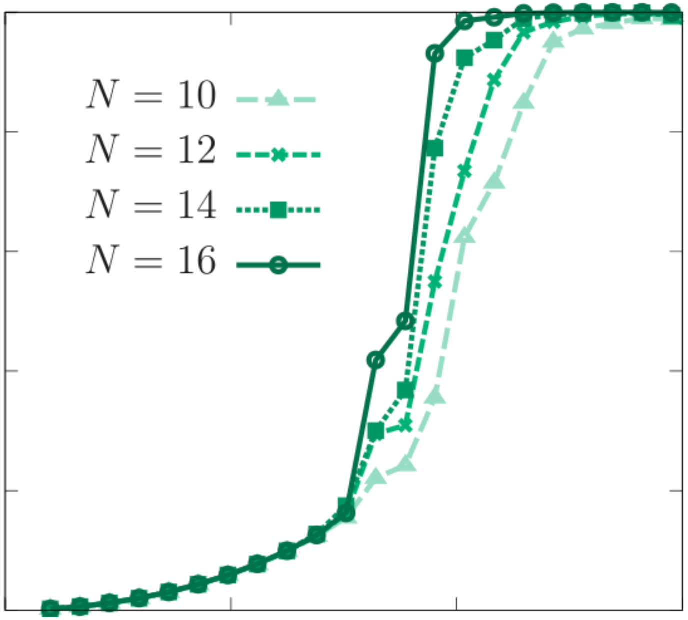
Period: $\tau = t/n$ ← small expansion parameter

Frequency: $\omega = \frac{2\pi}{\tau}$

Cold-atom context: e.g., Goldman and Dalibard, PRX 2014
Reviews: Eckardt 2016, Holthaus 2016

Classical analogue: Kaptiza's pendulum

https://youtu.be/rwGAzy0noU0



fast drive
stable

slow drive
unstable

Nice comparison classical/quantum:
D'Alessio, Polkovnikov, Ann. Phys. 2013

For small period $t/n = \tau$, effective Hamiltonian has a perturbative expansion (Magnus)

$$U^{(n)}(t) = \left[U_1\left(\frac{t}{n}\right)U_2\left(\frac{t}{n}\right)\cdots U_M\left(\frac{t}{n}\right)\right]^n = e^{-it\mathcal{H}(\tau)}$$

For small $t/n = \tau$ $$\mathcal{H}(\tau) = H + i\frac{\tau}{2}\sum_{l>m}[H_l, H_m] + \mathcal{O}(\tau^2),$$

Lloyds bound

$$U(t) - U^{(n)}(t) = \frac{t^2}{2n}\sum_{l>m=1}^{M}[H_l, H_m] + \mathcal{O}\left(\frac{t^3}{n^2}\right)$$

Cold-atom context: e.g., Goldman and Dalibard, PRX 2014
Reviews: Eckardt 2016, Holthaus 2016

Magnus expansion ensures energy localization

D'Alessio and Polkovnikov, Annals of Physics 2013

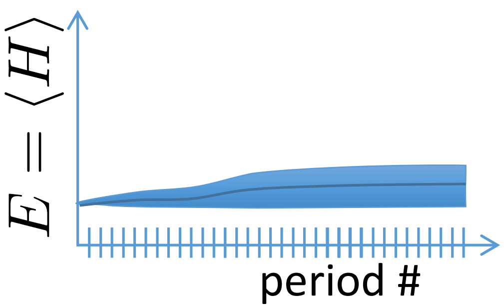
$$U^{(n)}(t) = e^{-it\mathcal{H}(\tau)} \qquad \mathcal{H}(\tau) = H + i\frac{\tau}{2}\sum_{l>m}[H_l, H_m] + \mathcal{O}(\tau^2),$$

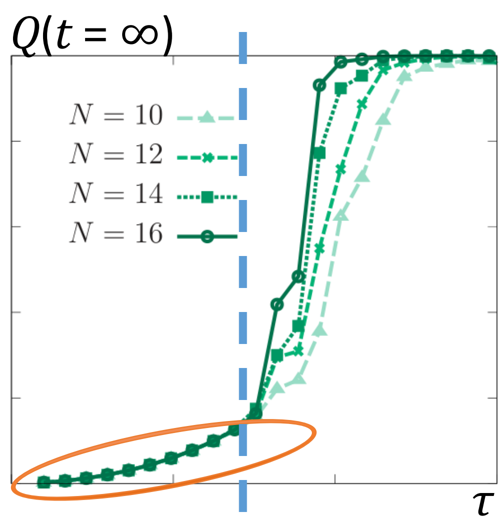
Zeroth order = time average = target H
→ emergent constant of motion

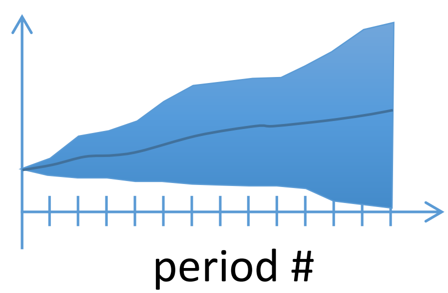
For small τ :
permits perturbation theory

large frequency /
small Trotter step $\tau = t/n$

small frequency /
large Trotter step τ





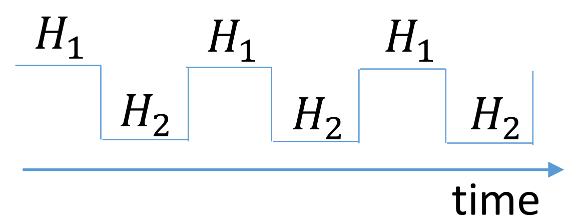


Energy localization enables linear response theory

Periodic sequence of two gates H_1, H_2

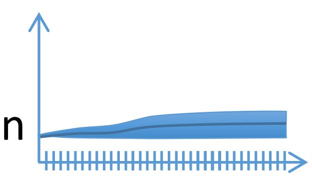
$$H(t) = \tfrac{1}{2}(H_1 + H_2) + \tfrac{1}{2}\,\text{square wave} * (H_1 - H_2)$$

perturbation at frequency $\omega = \frac{2\pi}{\tau}$



Main assumption of LRT:
state remains close to unperturbed state
Kubo 1962

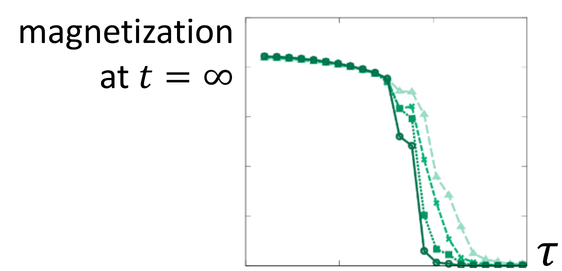
ensured by
energy localization



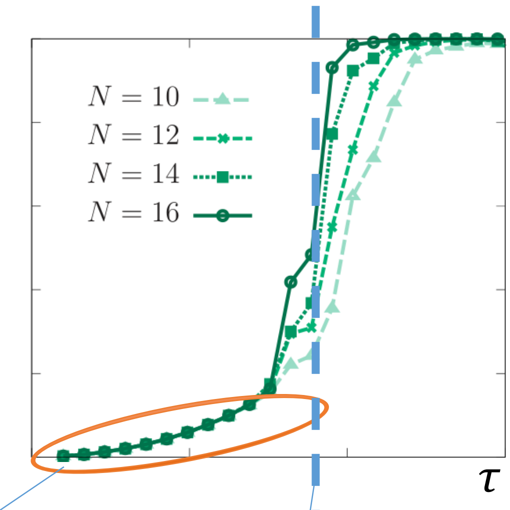
Consequence:
observables deviate only perturbatively

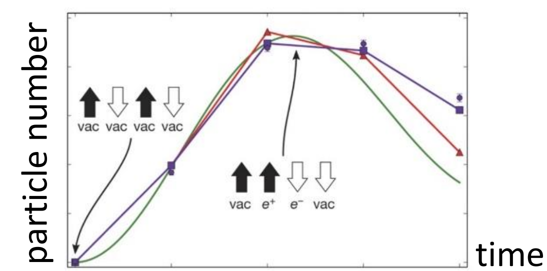
$$\Delta B(t) = B_\tau(t) - B_{\tau=0}(t)$$

$$\Delta B(\infty) = -i\tfrac{\tau}{4}\mathrm{Tr}(\rho_0[B, H_2 - H_1])$$



From these analytical arguments, we understand very well the perturbative regime





Martinez et al., Nature 2016

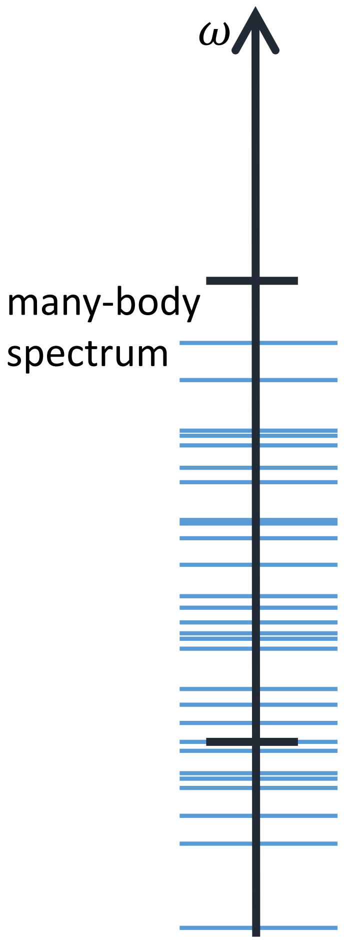
If the system is energy localized, this regime is robust

Challenge:
Predict breakdown point

$$\mathcal{H}(\tau) = H + i\frac{\tau}{2}\sum_{l>m}[H_l, H_m] + \mathcal{O}(\tau^2),$$

D'Alessio and Polkovnikov, Ann. Phys. 2013
D'Alessio and Rigol, PRX 2014
Lazarides, Das, and Moessner, PRE 2014
Ponte, Papic, Huveneers, and Abanin, PRL 2015
Bukov, Heyl, Huse, and Polkovnikov, PRB 2016
. . .

There may be three different regimes



$\omega \gg \Sigma \|H_l\|$

Perturbative response

No heating at large times

$$\Sigma \|H_l\| > \omega \gg \left| \frac{\langle \lambda | [H_m, H_n] | \lambda' \rangle}{E_\lambda - E_\lambda{}'} \right|, \qquad \forall \lambda, \lambda', m, n$$

Perturbative at low order, break down at higher orders possible

At most logarithmic heating over time (we do not see this)

Abanin, Roeck, and Huveneers, PRL 2015

$$\omega \not\gg \left| \frac{\langle \lambda | [H_m, H_n] | \lambda' \rangle}{E_\lambda - E_\lambda{}'} \right|$$

Non-perturbative; infinite heating

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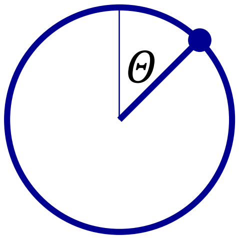
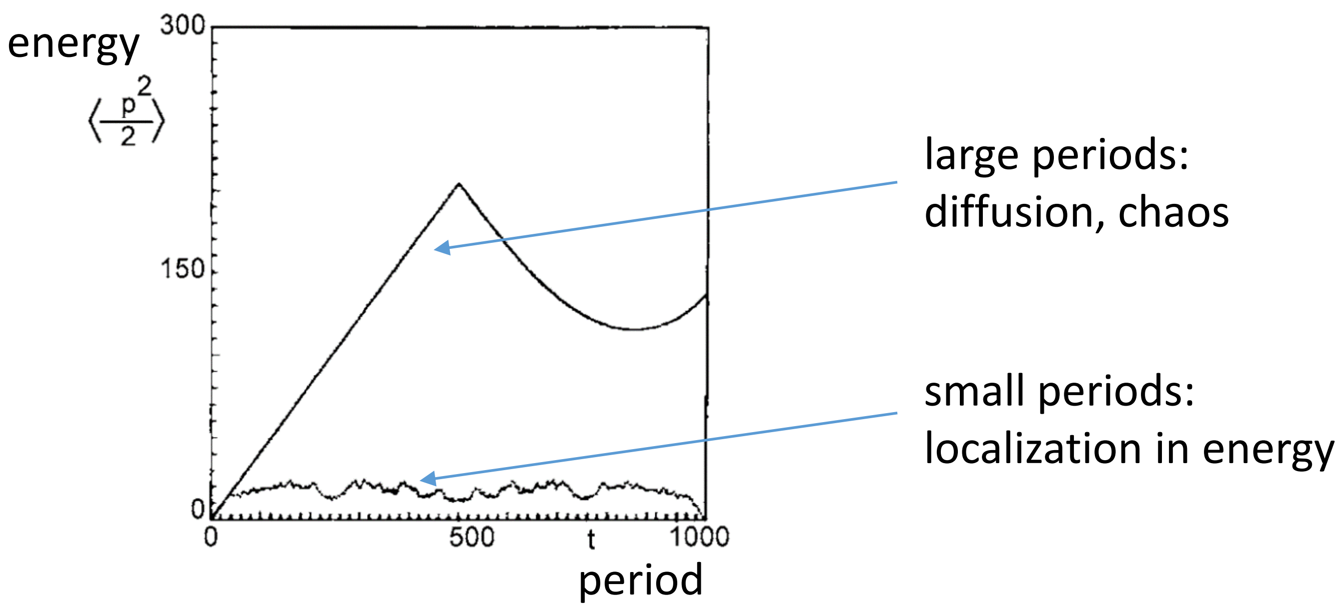
Transition to quantum chaos in periodically driven single-particle systems

See book Fritz Haake

Kicked rotor $H(t) = \frac{p^2}{2I} + \lambda \frac{I}{\tau} V(\Theta) \sum_{n=-\infty}^{+\infty} \delta(t - n\tau)$





Break-down as transition of Floquet Hamiltonian to quantum chaos

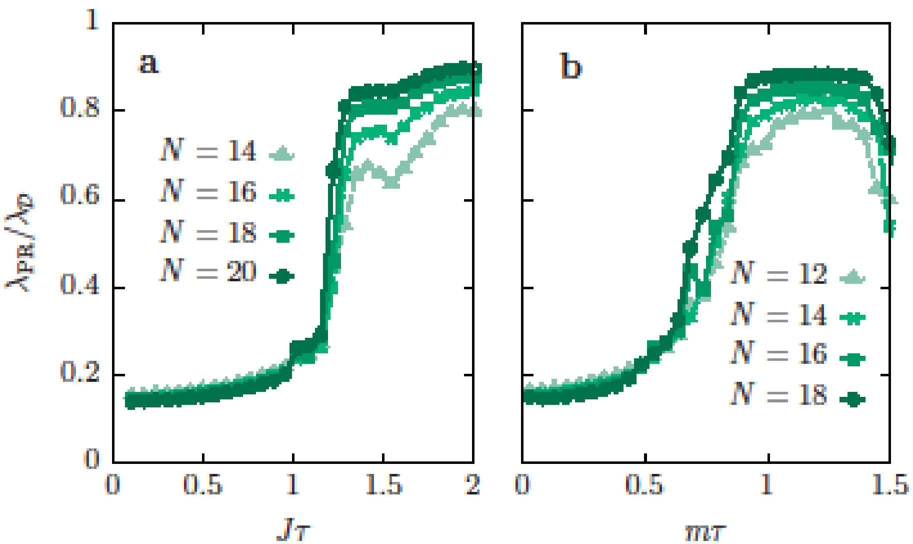
Floquet Hamiltonian $$U^{(1)} = \left[U_1\left(\frac{t}{n}\right)U_2\left(\frac{t}{n}\right)\cdots U_M\left(\frac{t}{n}\right)\right] = e^{-i\,H_F\,\tau}$$

NB: eigenvalues follow Wigner-Dyson statistics for all τ (for generic ideal H)

Characterize chaos through spread over Floquet basis states

$$\mathrm{PR} = \Sigma|\langle\psi_0|\varphi_\nu\rangle|^4 \qquad \lambda_{\mathrm{PR}} = -\log(\mathrm{PR})/\mathrm{N}$$

$|\varphi_\nu\rangle$ = eigenstates of Floquet Hamiltonian



all basis states are equally likely

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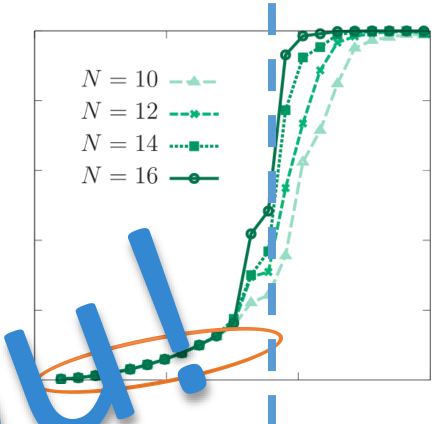
Digital quantum simulators are more robust than one may think (for local observables)

Sharp threshold, connected to quantum chaos



We understand the perturbative behavior from periodically driven systems and LRT

Valid also for Trotter on classical computers (e.g. tensor networks)

Thank you!

Paper in preparation!