Quantum-Classical Hybrid Monte Carlo Algorithm with Applications to AQC

Itay Hen
Information Sciences Institute, USC

Workshop on Theory and Practice of
AQC and Quantum Simulation
Trieste, Italy
August 23, 2016

Joint work with **Tameem Albash**
and Gene Wagenbreth

Information Sciences Institute
USC School of Engineering

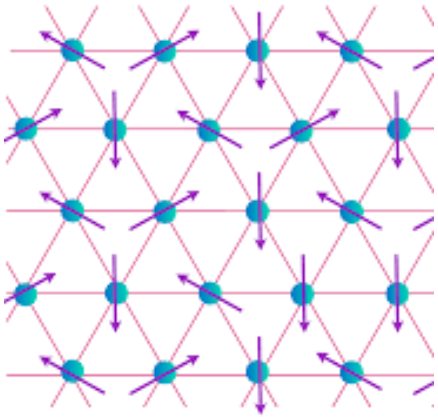
Outline

- motivation
- a different decomposition of the quantum partition function
- quantum-classical Monte Carlo algorithm
- some (preliminary) results
- applications to AQC
- conclusions and outlook

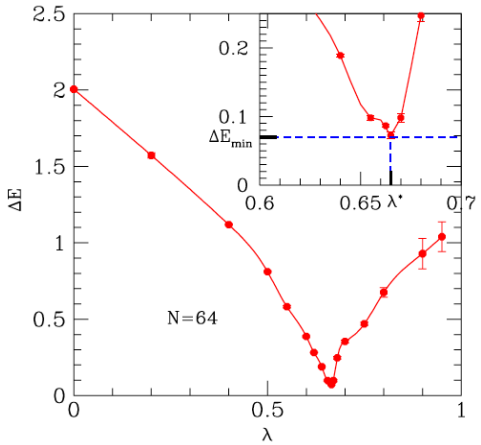
Motivation

Motivation

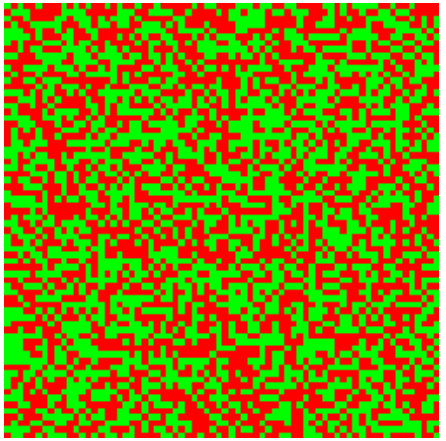
- for most large quantum many body systems, quantum Monte Carlo (QMC) is the only approach to get any results.
- still, QMC is inefficient under certain circumstances.



sign problem
(negative weights)



small energy gaps
(phase transitions)

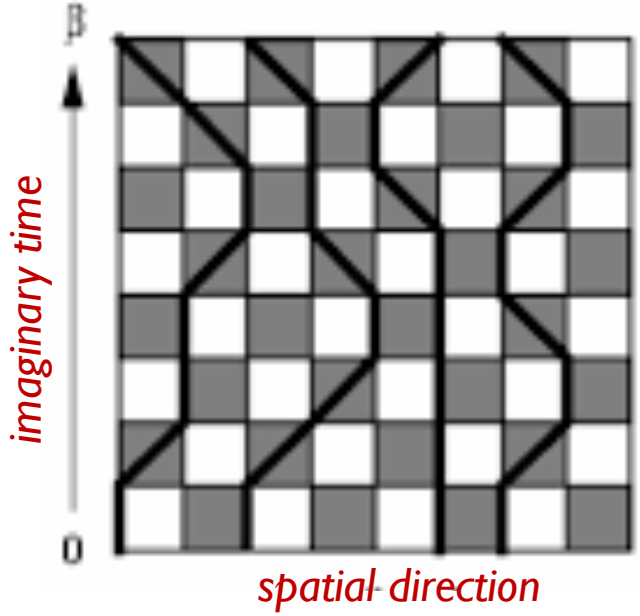


classical glassiness

- quantum many-body systems that are almost classical tend to freeze: quantum fluctuations driving the simulations are too small but algorithms do not properly converge to thermal classical algorithms.

Standard methods

- path integral Monte Carlo methods are prone to Trotterization errors.
- at low temperatures (high β), imaginary time slices must be made smaller and smaller, leading to low acceptance rates of updates.
- other schemes are immune to Trotterization errors:
  - continuous-time Monte Carlo [Prokof'ev et al].
  - stochastic series expansion (SSE) [Sandvik].
- these however too have other issues.



Standard stochastic series expansion

- SSE: no Trotterization. first, the trace in the partition functions is replaced by an explicit sum over computational basis states:

$$Z = \mathrm{Tr}\left[e^{-\beta H}\right] = \sum_{\{z\}} \langle z|e^{-\beta H}|z\rangle$$

- then, in lieu of slicing β, one Taylor-expands the exponent

$$Z = \sum_{z} \sum_{n=0}^{\infty} \frac{\beta^n}{n!} \langle z|(-H)^n|z\rangle$$

- as a next step, the Hamiltonian is written as a sum of local operators.

$$H = -\sum_{j} H_j \qquad \text{where} \qquad H_j|z\rangle \sim |z'\rangle$$

some of those are diagonal, some are off-diagonal.

Standard stochastic series expansion

- the partition function can then be written as a triple sum of weights:

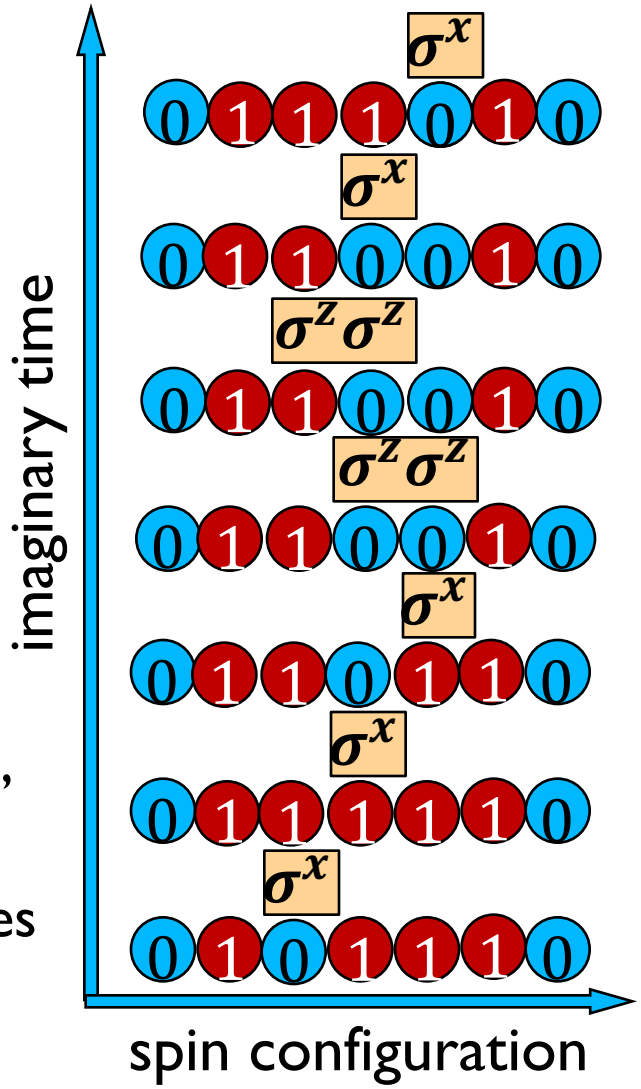
$$Z = \sum_{z} \sum_{n=0}^{\infty} \sum_{\{S_n\}} \frac{\beta^n}{n!} \langle z|S_n|z\rangle$$

where $\{S_n\}$ is the set of all products of local operators H_j of size *n*:

$$S_n = H_{j_1} H_{j_2} \cdots H_{j_n}$$

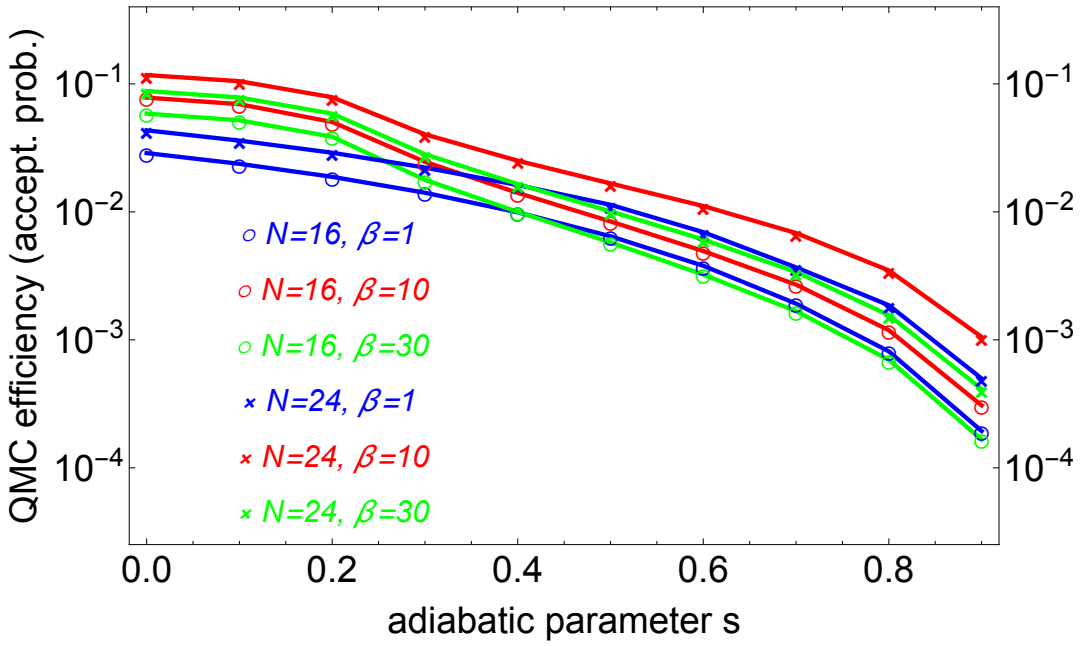
- to interpret $\frac{\beta^n}{n!}\langle z|S_n|z\rangle$ as weights, the diagonal operators must have positive eigenvalues, which creates a (curable) diagonal sign problem. constants must be added to rectify that. sometimes significantly affects the efficiency of the algorithm.

a typical segment of a QMC configuration



Issues with standard SSE

- for many systems, SSE is found to be very effective (e.g., the Bose-Hubbard model). good global update moves.
- for other systems such as the transverse field Ising model, there's the possibility of `freeze-out' inside the glassy phase.
- if quantum fluctuations are small, they do not appear often enough to generate new configurations with plausible acceptance rates.
- some sort of percolation threshold.
- can this freezing be cured?



A different decomposition of the quantum partition function

A different decomposition

- what if we do not break apart the classical part?

  let us write the Hamiltonian as a diagonal (highly non-local) operator and a sum of local off-diagonal operators:

$$H = H_{\text{classical}} + \sum_j t_j \cdot V_j$$

- initially proceed with standard SSE approach.

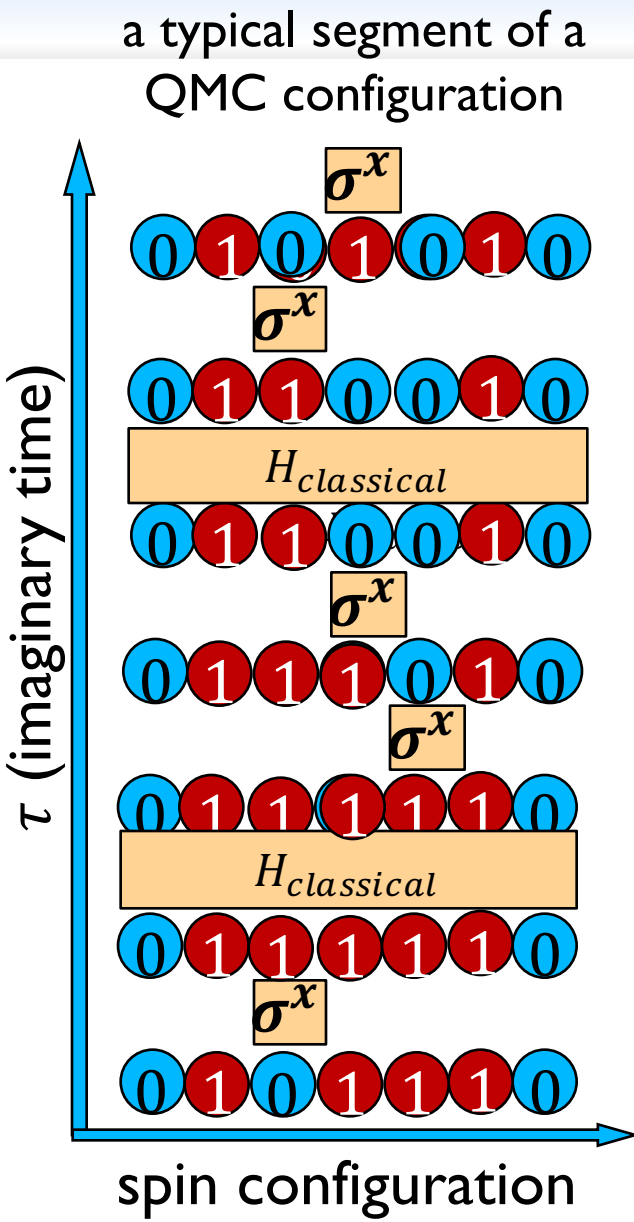
  we still obtain sequences of the form:

$$S_n = H_{j_1} H_{j_2} \cdots H_{j_n}$$

- now however the operators are

$$H_j = \begin{cases} H_{\text{classical}} & \text{diagonal, non-local} \\ t_j V_j & \text{off-diagonal, local} \end{cases}$$

- since the operators are non-local, standard SSE does not work (acceptance rates are low).



A different decomposition

- in the new formalism, we proceed by evaluating all the diagonal $H_{\text{classical}}$ operators inside the products:

$$\langle z|S_n|z\rangle = \langle z|\, H_{j_1}\, H_{j_2}\, \cdots\, H_{j_n}\, |z\rangle$$

$$\langle z_0| \rightarrow \langle z_1| \rightarrow \langle z_1| \cdots\cdots\rightarrow \langle z_n|$$

- the off-diagonal terms modify the classical configurations.
- the diagonal terms each generate a factor of classical energy

$$H_{\text{classical}}|z\rangle = E_c(z)|z\rangle$$

that can be pulled out of the bra-ket.

A different decomposition

- the next step is: group together of all `standard SSE' weights $\langle z|S_n|z\rangle$ that have the same 'off-diagonal backbone' :

$$\langle z|S_q|z\rangle = \langle z|\, V_{j_1}\, V_{j_2}\, \cdots\, V_{j_q}\, |z\rangle$$

- this gives (for simplicity we set $t_j = t$):

$$Z = \sum_z \sum_{n=0}^{\infty} \sum_{\{S_n\}} \frac{\beta^n}{n!} \langle z|S_n|z\rangle = \sum_z \sum_{q=0}^{\infty} \sum_{\{S_q\}} (-t)^q \langle z|S_q|z\rangle$$

$$\times \left(\sum_{n=q}^{\infty} \frac{\beta^n (-1)^{n-q}}{n!} \sum_{\sum k_i = n-q} E_c^{k_0}(z_0) \cdot \ldots \cdot E_c^{k_q}(z_q) \right)$$

$$E_c(z_i) = \langle z_i|H_{\text{classical}}|z_i\rangle$$

- formally, this is a sum of infinitely many terms.

A different decomposition

- as it turns out, this *infinite sum*

$$\left(\sum_{n=q}^{\infty} \frac{\beta^n (-1)^{n-q}}{n!} \sum_{\sum k_i = n-q} E_c^{k_0}(z_0) \cdot \ldots \cdot E_c^{k_q}(z_q) \right) =$$

can be regrouped to give

$$e^{-\beta [E_0, \ldots, E_q]}$$

this is the *divided difference* of the Boltzmann factor of *sequences* (multi-sets) of intermediate classical energies along the imaginary time direction.

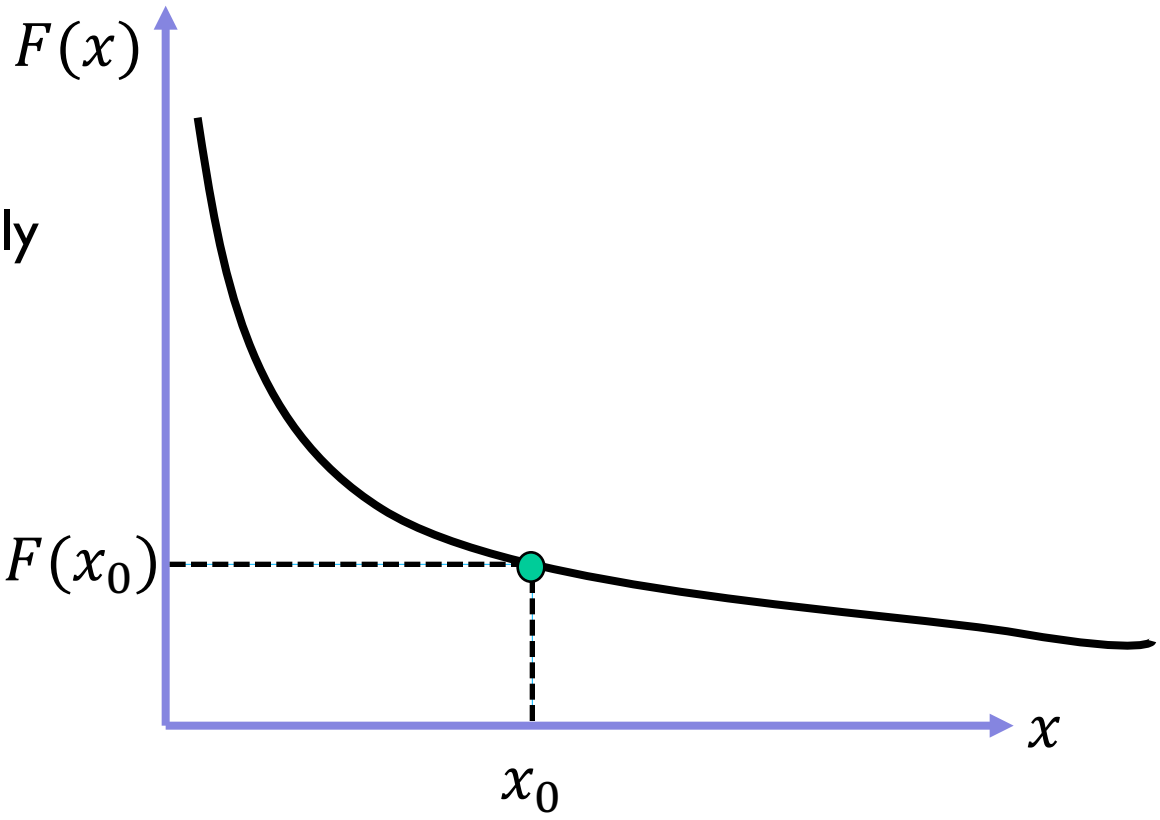
Digression: divided differences

- the divided differences of a function $F(x)$ with respect to the input multi-set $[x_0, \ldots x_q]$ is given by:

$$F([x_0, \ldots, x_q]) \equiv \sum_{j=0}^{q} \frac{F(x_j)}{\prod_{k \neq j}(x_j - x_k)}$$

- the divided difference of a function with an input multi-set of size one, is simply

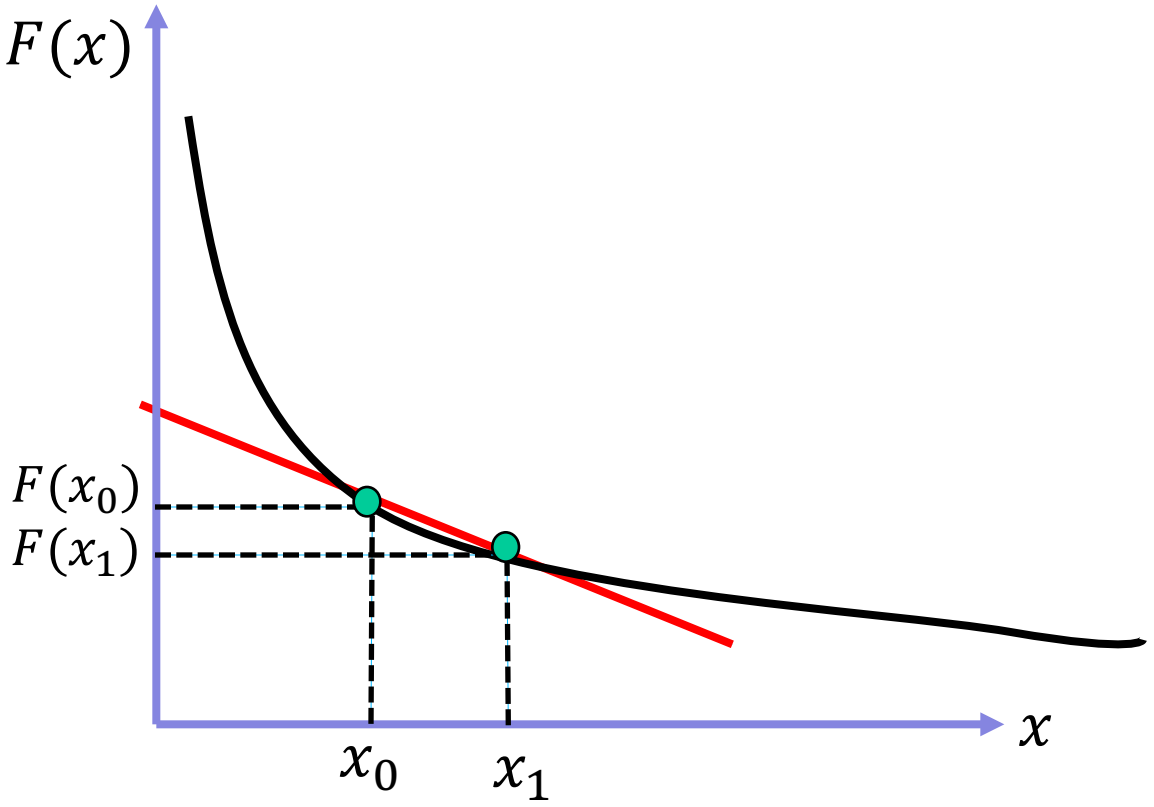
$$F[x_0] = F(x_0)$$



Digression: divided differences

- the divided differences of a function taking as input a multi set with two elements is:

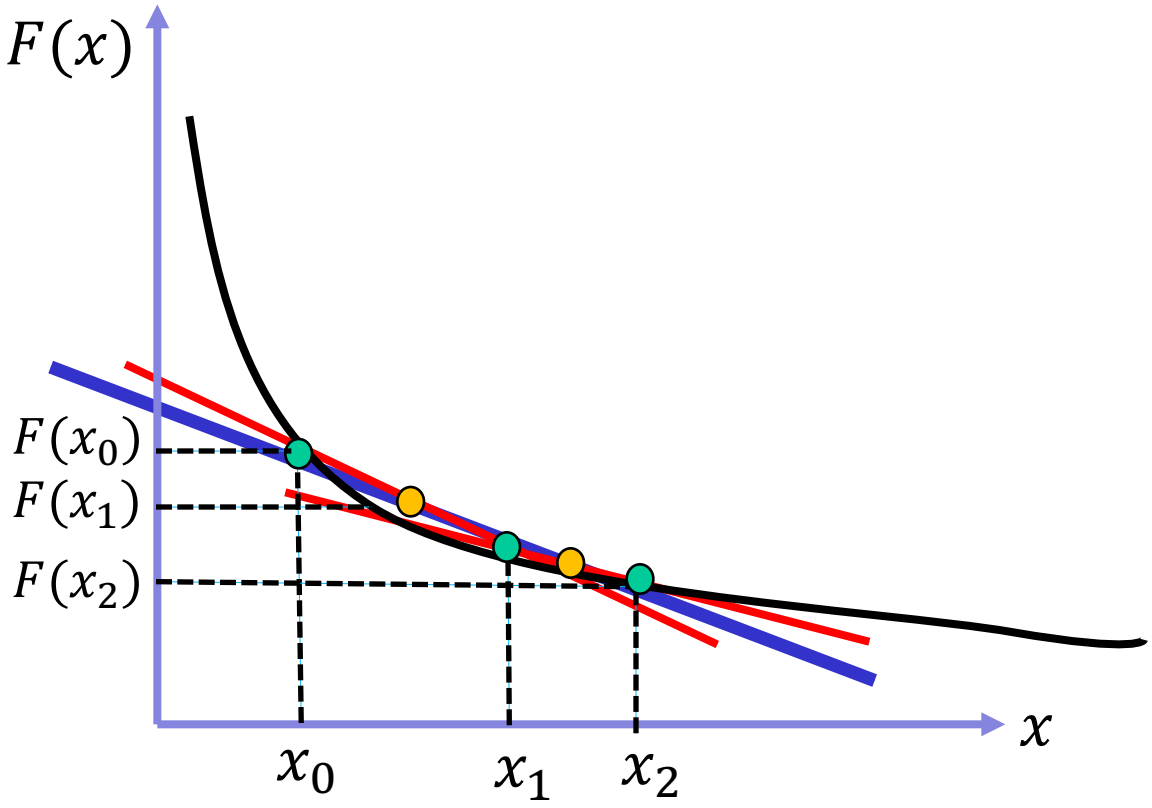
$$F[x_0, x_1] = \frac{F(x_1) - F(x_0)}{x_1 - x_0} \approx F'(\xi)$$



Digression: divided differences

- the divided differences of a function taking as input a multi set with three elements is:

$$F[x_0, x_1, x_2] = \frac{F[x_0, x_1] - F[x_1, x_2]}{x_0 - x_2} \approx \frac{1}{2} F''(\xi)$$



Digression: divided differences

- in the general case, the evaluation of the divided differences of a function with $q+1$ inputs

$$F([x_0,\ldots,x_q]) \equiv \sum_{j=0}^{q} \frac{F(x_j)}{\prod_{k\neq j}(x_j - x_k)}$$

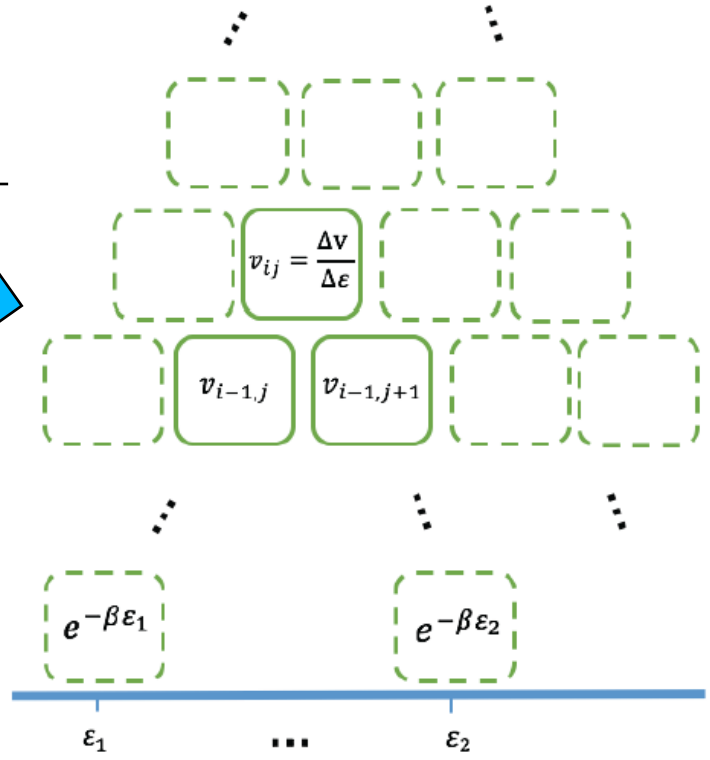
is done via the recursion relation:

$$F[x_0,\ldots,x_q] = \frac{F[x_0,\ldots,x_{q-1}] - F[x_1,\ldots,x_q]}{x_0 - x_q}$$

- also:

$$F[x_0,\ldots,x_q] = \frac{F^{(n)}(\xi)}{n!}$$

- the computational cost of calculating this infinite sum scales as q^2 in the worst case.



Final form of partition function

- in terms of divided differences of the Boltzmann factor, the partition function ends up looking like:

$$Z = \sum_{z} \sum_{q=0}^{\infty} \sum_{\{S_q\}} \langle z|S_q|z\rangle t^q e^{-\beta[E_0,\ldots,E_q]}$$

note! $\langle z|S_q|z\rangle = \langle z|z'\rangle = \delta_{z,z'}$. we can therefore simply write:

$$Z = \sum_{z} \sum_{\{S_q:\langle z|S_q|z\rangle \neq 0\}} t^q e^{-\beta[E_0,\ldots,E_q]}$$

Z is therefore a series expansion of `generalized Boltzmann weights' with respect to the quantum strength parameter t.

Generalized Boltzmann weights

- as a series in the `quantumness parameter' t, the partition function can be written as:

$$Z = \sum_z e^{-\beta H_{\text{classical}}(z)} + t^2 \sum_{\{S_2 : \langle z|S_2|z\rangle \neq 0\}} e^{-\beta[E_0, E_1, E_0]} + \dots$$

- if the quantum parameter is zero, the partition function decomposition reduces to that of the classical one:

$$t^q e^{-\beta[E_0,\dots,E_q]}\big|_{q=0} = e^{-\beta E_0} = e^{-\beta E_c(z)}$$

Generalized Boltzmann weights

- interim summary: we have a decomposition of the partition function of the form

$$Z = \sum_{\{c\}} W_c \qquad \text{where} \quad c = (|z\rangle, S_q)$$

a product of off-diagonal operators

classical state

- the weights are: $W_c = t^q e^{-\beta[E_0,\ldots,E_q]}$
- the sequence (multi-set) of energies $[E_0, E_1, \ldots, E_q]$ is generated by the action of the sequence S_q on the classical state $|z\rangle$:

$$\langle z|S_q|z\rangle = \langle z|\, V_{j_1}\, V_{j_2}\, \cdots\, V_{j_q}\, |z\rangle$$

$$\langle z_0| \to \langle z_1| \to \langle z_2| \cdots\cdots \to \langle z_q|$$

$$E_c(z_0)\ E_c(z_1)\ E_c(z_2)\ \ldots\ E_c(z_q)$$

Generalized Boltzmann weights

- other interesting properties of the GBWs:
  - always positive for systems with no sign problem.
    never a `diagonal sign problem'. no artificial parameters required.
  - doesn't solve the sign problem.
  - invariance of weight ratios under a constant energy shift:

$$e^{-\beta[E_0+\Delta E,\ldots,E_q+\Delta E]} = e^{-\beta\Delta E} e^{-\beta[E_0,\ldots,E_q]}$$

  - a connection to continuous-time MC via the
    Hermite-Genocchi formula

$$e^{-\beta[E_0,\ldots,E_q]} = \int_\Omega \mathrm{d}t_0 \ldots \mathrm{d}t_q e^{-\beta(E_0 t_0 + E_1 t_1 + \ldots + E_q t_q)}$$

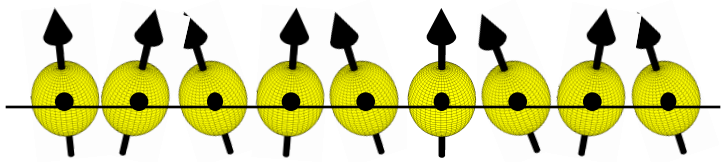
with Ω: $t_i \geq 0, \Sigma t_i = 1$

Quantum-classical Monte Carlo algorithm

A trivial example first:

- consider the case of the "off-diagonal" Hamiltonian:

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



- here, the partition function is:

$$Z = \sum_q t^q \sum_{\{z\}} \sum_{\{S_q\}} \langle z|S_q|z\rangle e^{-\beta[E_0,\ldots,E_q]}$$

with classical energies $E_0 = \cdots = E_q = 0$

- in this case $e^{-\beta[E_0,\ldots,E_q]} = \dfrac{(-\beta)^q}{q!}$
- so the partition function reduces to

$$Z = 2^N \sum_q \frac{(-\beta)^q t^q}{q!} N_p(q) \qquad \text{with} \quad N_p(q) = \frac{1}{2^N}\sum_{k=0} \binom{N}{k} (N-2k)^q$$

being the number of nonzero weights per size q

- evaluates to the correct expression: $Z = (2\cosh \beta t)^n$

Quantum-classical Monte Carlo algorithm

- for more complicated systems, we can use the decomposition to form a quantum-classical MC algorithm.
- we generate a Markovian process on the configurations

$$c = (|z\rangle, S_q)$$

classical state — $|z\rangle$

a product of local off-diagonal operators — S_q

- initial configuration: the empty product, i.e., $S_q = 1$, and a randomly chosen classical state $|z\rangle$:

$$W_c = t^q e^{-\beta[E_0,\ldots,E_q]} \Rightarrow e^{-\beta E_0} = e^{-\beta E_c(z)}$$

this corresponds to starting with a classical system.

Quantum-classical Monte Carlo algorithm

- generic updates that mildly perturb the GBW:
  - a simple swap (changes S_q):

$$\langle z|V_{i_1} \dots V_{i_j} \overset{z'}{|} V_{i_k} \dots V_{i_q}|z\rangle \Leftrightarrow \langle z|V_{i_1} \dots V_{i_k} \overset{z''}{|} V_{i_j} \dots V_{i_q}|z\rangle$$

  - a block swap (changes $S_q, |z\rangle$):

$$\langle z|V_{i_1} \dots V_{i_j} \overset{z'}{|} V_{i_k} \dots V_{i_q}|z\rangle \Leftrightarrow \langle z'|V_{i_k} \dots V_{i_q} \overset{z}{|} V_{i_1} \dots V_{i_j}|z'\rangle$$

  - creation/annihilation (changes q, S_q):

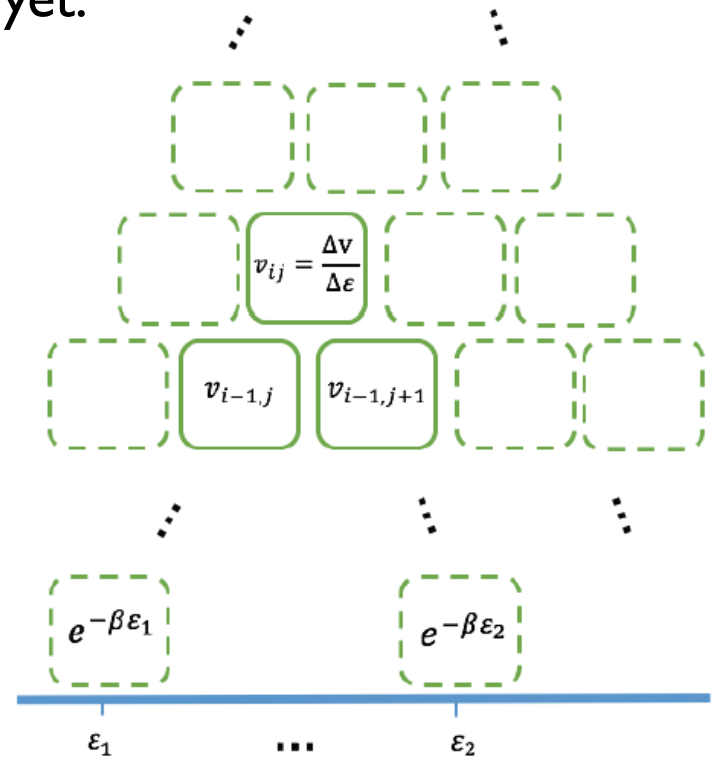
$$\langle z|V_{i_1} \dots V_{i_j} \overset{z'}{|} V_{i_k} \dots V_{i_q}|z\rangle \Leftrightarrow \langle z|V_{i_1} \dots V_{i_j} \overset{z''}{|} V V V_{i_j} V_{i_k} \dots V_{i_q}|z\rangle$$

  - classical moves (change $|z\rangle$):

$$\langle z|V_{i_1} \dots V_{i_j} V_{i_k} \dots V_{i_q}|z\rangle \Leftrightarrow \langle z'|V_{i_1} \dots V_{i_j} V_{i_k} \dots V_{i_q}|z'\rangle$$

Measurements and issues

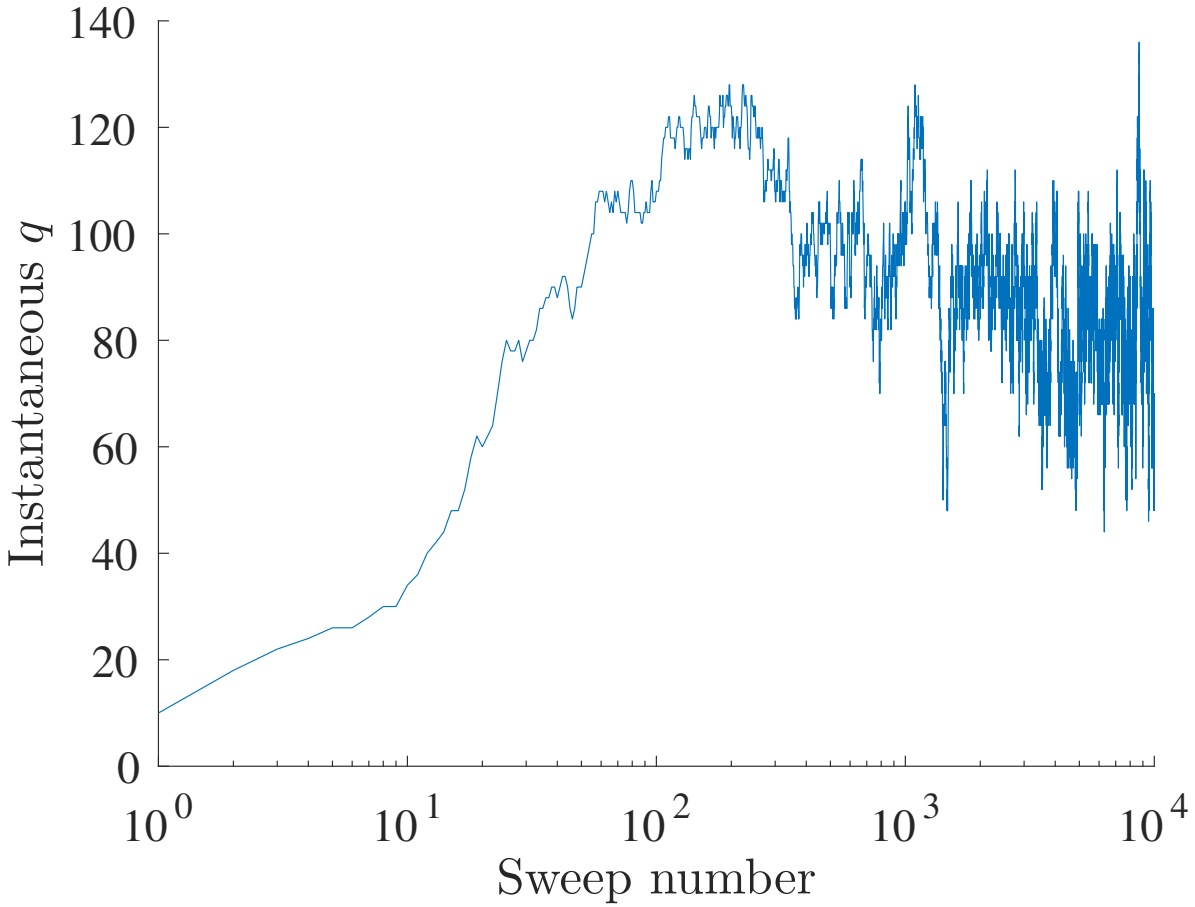
- measurements are easily done:
  - arbitrary diagonal operators.
  - thermal averages of off-diagonal operators and products thereof.
  - haven't worked out correlation functions yet.
- issues:
  - precision required for calculation of weights is high.
  - haven't figured out global updates yet.
  - weight calculation is somewhat costly requiring sometimes ~q operations. however corresponds to the sum of very many standard weights.



Some (preliminary) results

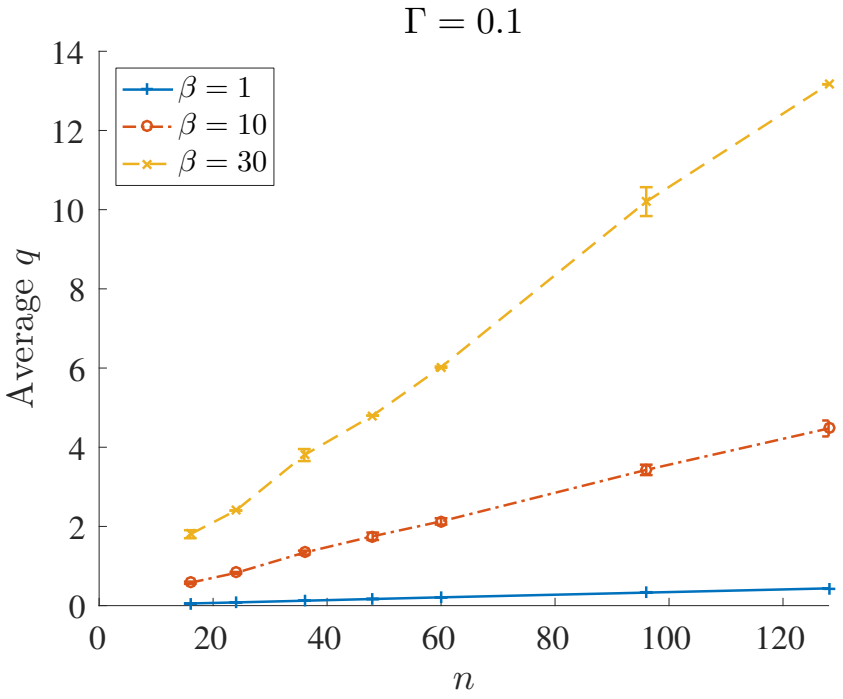
Dynamical imaginary time

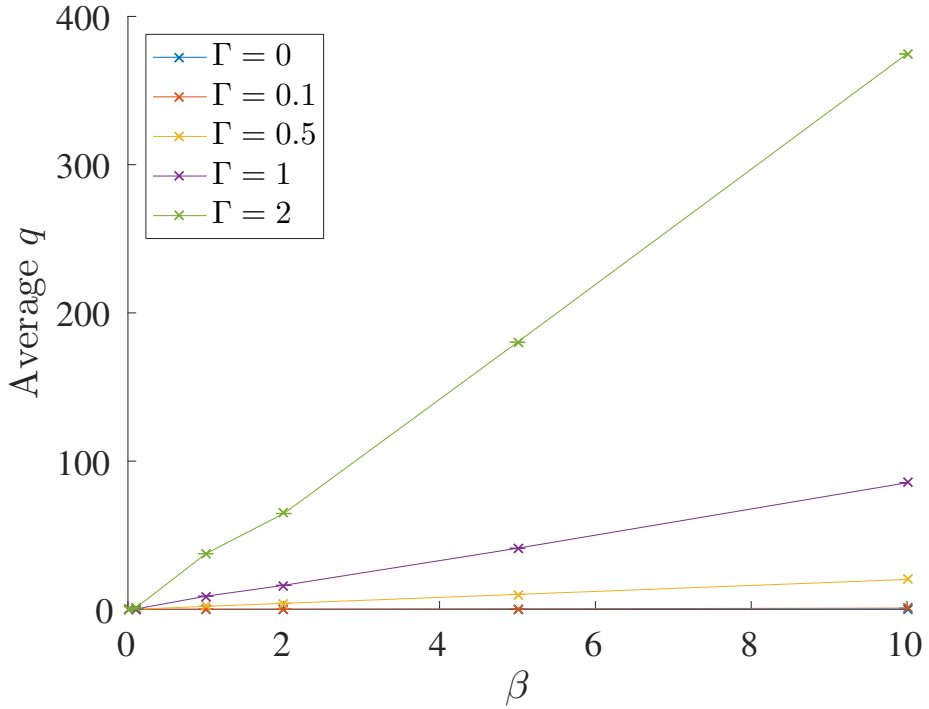
- the size of S_q, namely q, is the dynamical size of periodic imaginary time.
- q varies dynamically and levels off (but fluctuates) as the simulation evolves.
- remains zero for classical systems (probability for pair creation is zero).
- also, no Trotterization errors.



Dynamical imaginary time

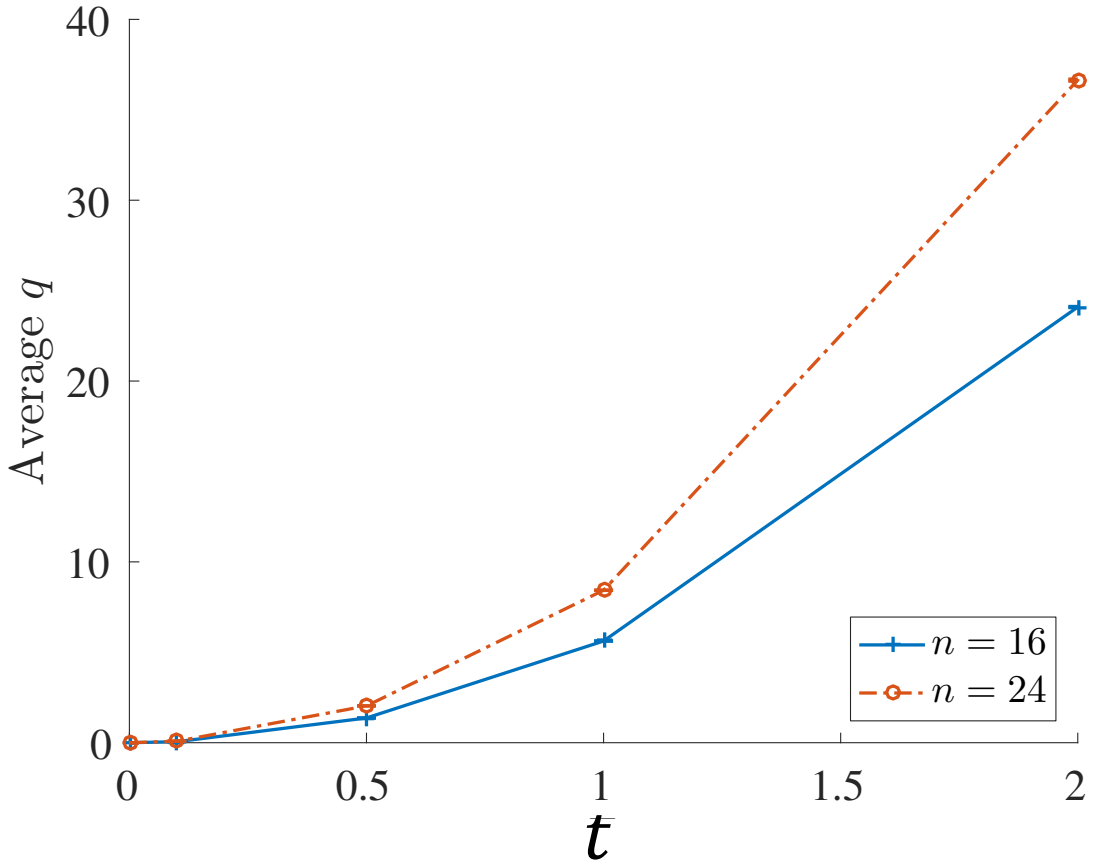
- size of imaginary time dimension:
  - $\langle q \rangle$ scales linearly with inverse temperature β and
  - $\langle q \rangle$ scales linearly with problem size n.





Dynamical imaginary time

- size of imaginary time dimension:
  - $\langle q \rangle$ grows with the "quantumness" (quadratically it seems).

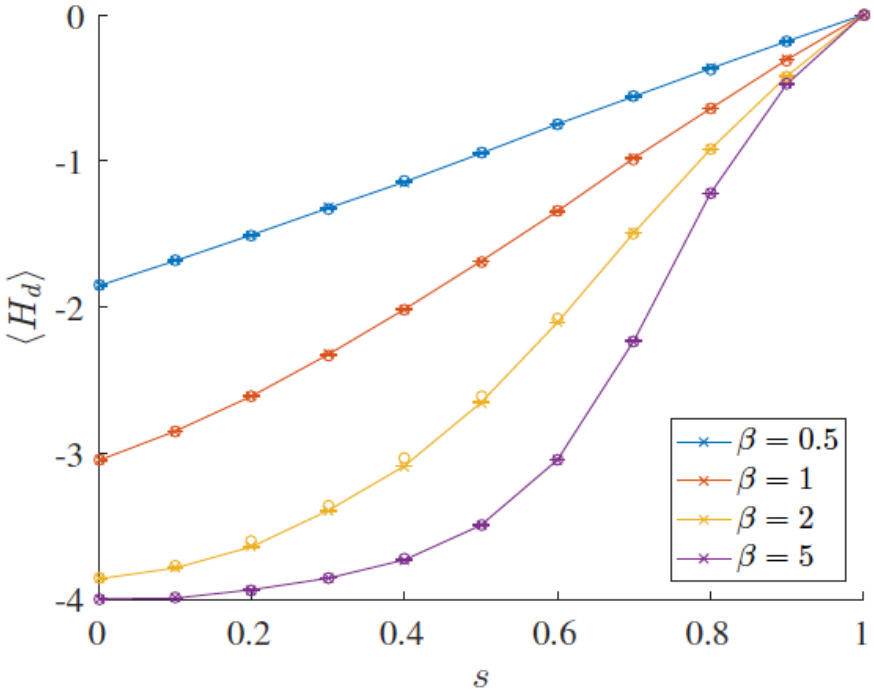


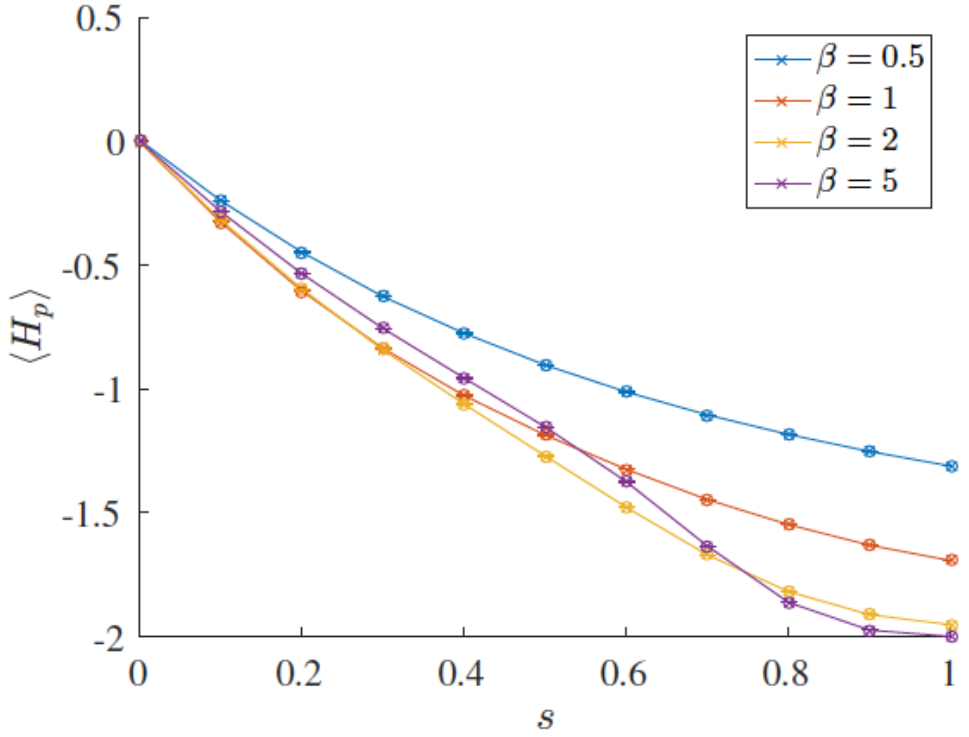
Preliminary results

- comparison against exact diagonalization.

$$H = s\sum_{\langle ij\rangle} J_{ij}\sigma_i^z\sigma_j^z + (1-s)\sum_i \sigma_i^z$$

- fully connected anti-ferromagnet. system size is $n = 16$.



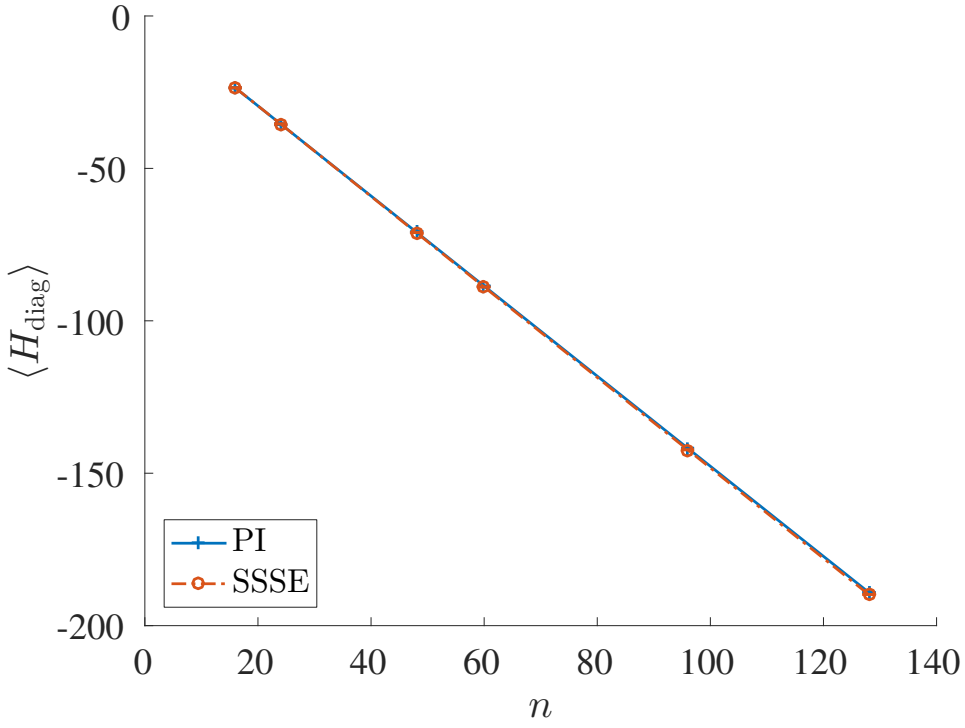


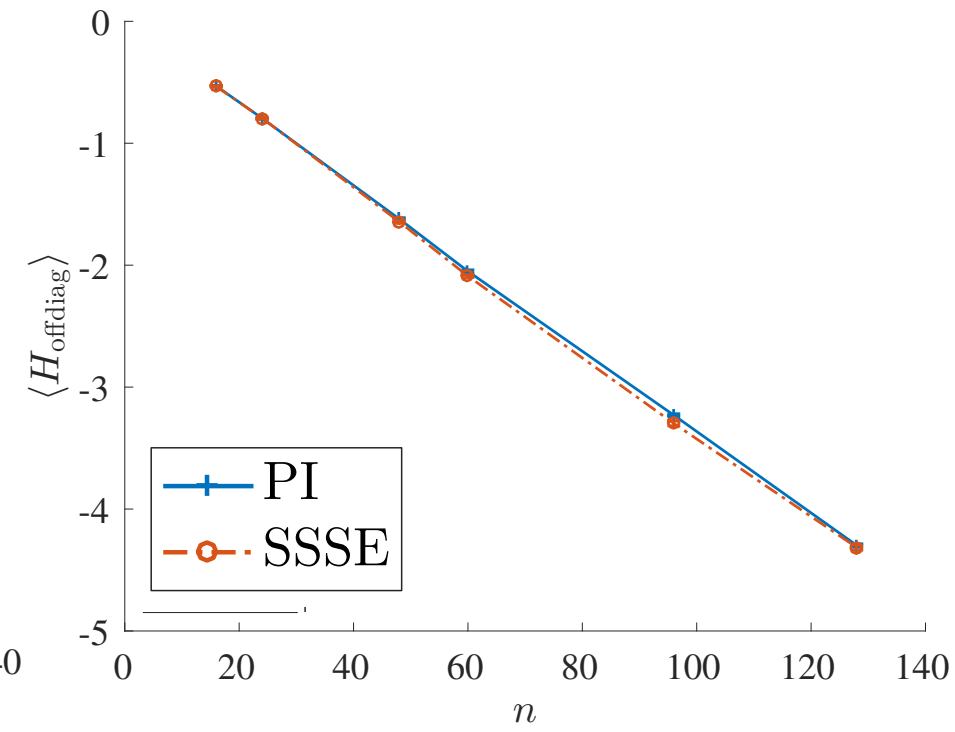
Preliminary results

- comparison against path integral MC.

$$H = \sum_{\langle ij \rangle} J_{ij} \sigma_i^z \sigma_j^z + t \sum_i \sigma_i^z$$

- instances are random 3-regular max-2-sat. here, $t = 0.1$ ("mostly" classical).

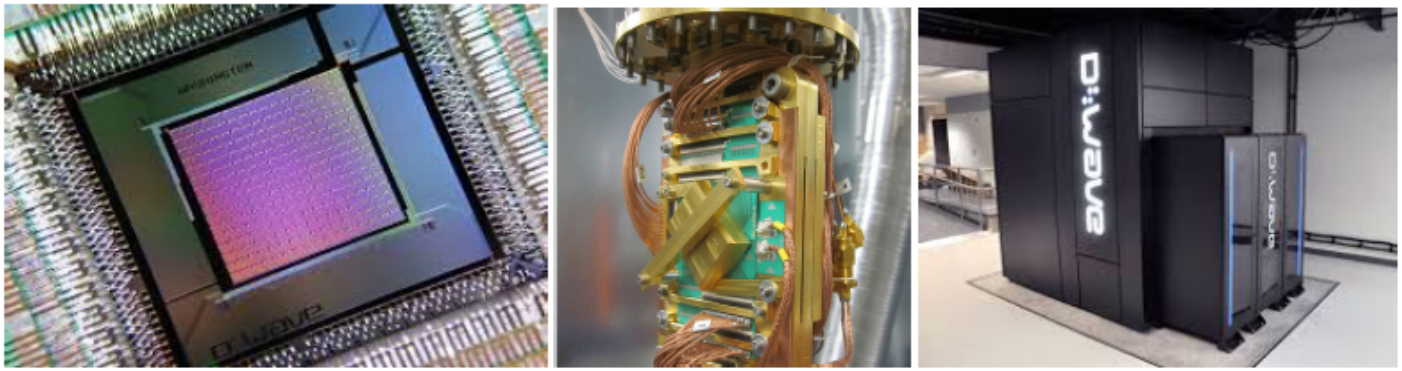




Applications to AQC

Applications to AQC

- experimental quantum annealers



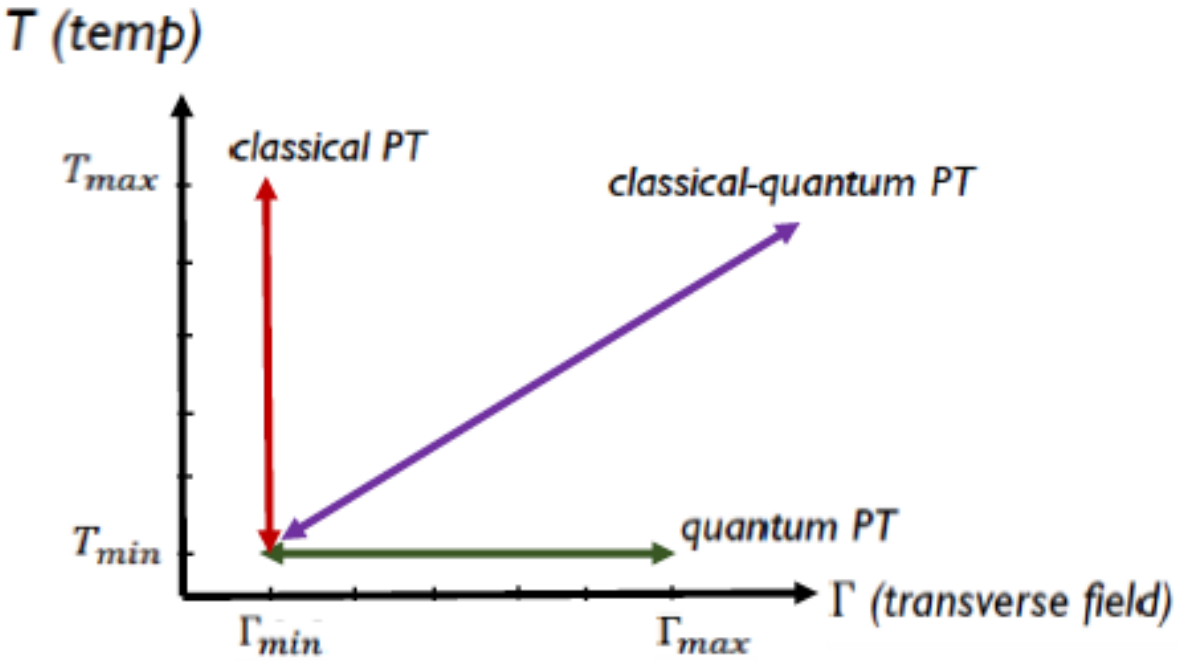
that implement the transverse-field Ising model:

$$H = \sum_{\langle i,j \rangle} J_{ij}\sigma_i^z\sigma_j^z + \sum_j h_j\sigma_j^z - t\sum_j \sigma_j^x$$

- explore the full spectrum of purely quantum to purely classical dynamics.
- trace curves in the quantum-classical, or transverse field-temperature, parameter space.

Applications to AQC

- may benefit from such quantum-classical MC method.
- for example quantum-classical parallel tempering which would mimic experimental quantum annealers.
- bridges quantum and classical (thermal) evolution in a natural way.



Conclusions and outlook

Conclusions and outlook

- preliminary results are positive.
- technique is “clean”; has no free parameters whatsoever.
- more work to be done.
- decomposition of the partition function seems to indicate certain important ”natural” qualities.
- perhaps this decomposition of the quantum partition function may be useful in other applications.
- connection to continuous-time QMC should be resolved.
  some indications of a profound relation.

Thank You!

Quantum-Classical Hybrid Monte Carlo Algorithm with Applications to AQC

Itay Hen
Information Sciences Institute, USC

Workshop on Theory and Practice of
AQC and Quantum Simulation
Trieste, Italy
August 23, 2016

Joint work with **Tameem Albash**
and Gene Wagenbreth

Information Sciences Institute
USC School of Engineering