Complexity of quantum impurity problems

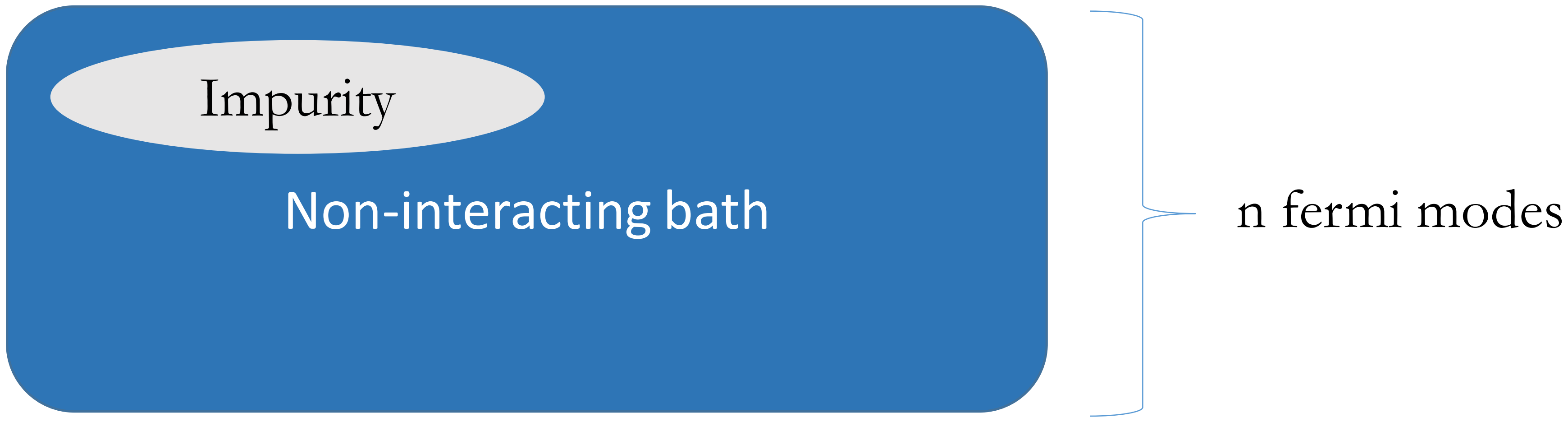
Sergey Bravyi

David Gosset

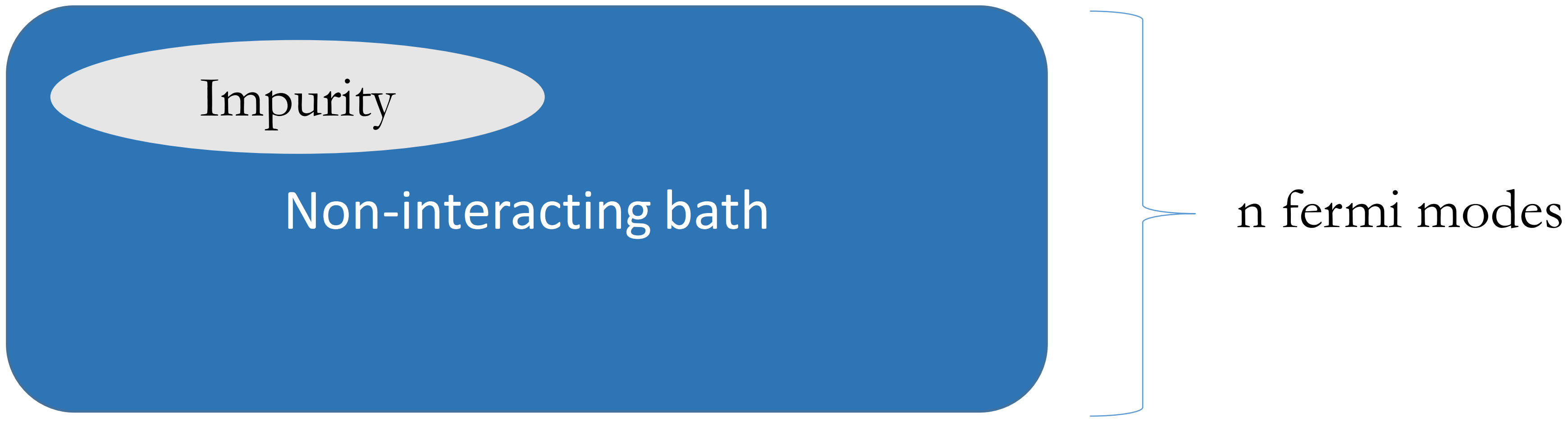
IBM

arXiv:1609.00735

A quantum impurity model describes a free fermion bath coupled to a small but strongly interacting impurity.



A quantum impurity model describes a free fermion bath coupled to a small but strongly interacting impurity.



$$H = H_{bath} + H_{imp}$$

Non-interacting
(quadratic)

Acts nontrivially
on $m = O(1)$ fermi modes

Quantum impurity models were introduced to study the Kondo effect:

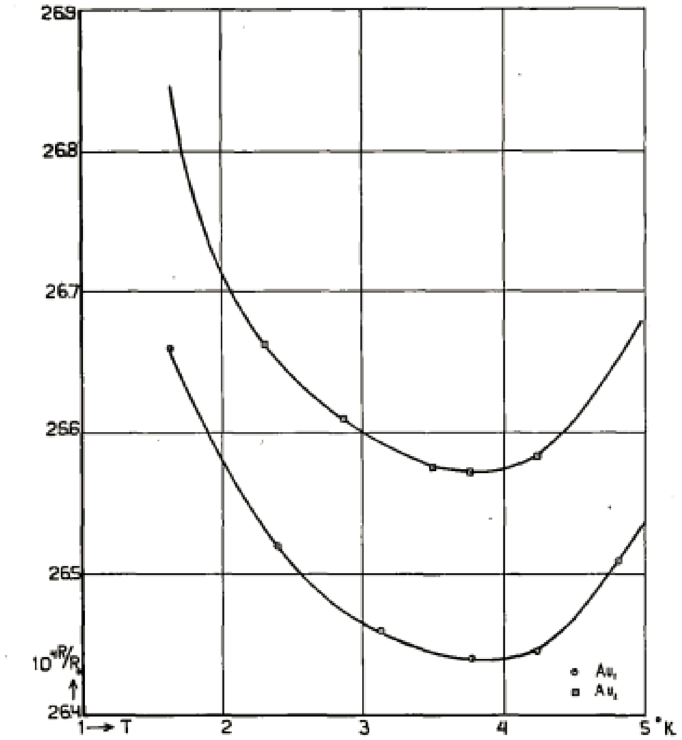


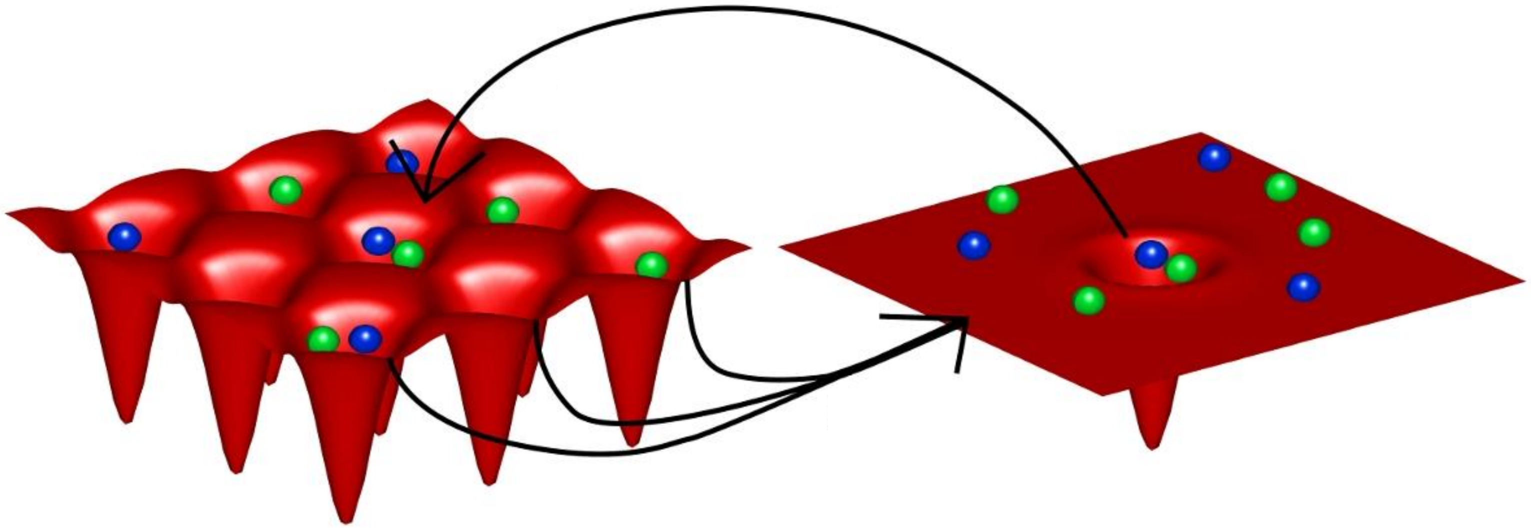
Fig. 1. Resistance of *Au* between 1°K. and 5°K.

"The resistance curve of the gold wires measured (not very pure) has a minimum"

W.J de Haas, J. de Boer, and G.J van den Berg
Physica 1, 1115 (1933)

[Anderson 1961, Kondo 1964, Wilson 1975]

Dynamical Mean Field Theory (DMFT): A quantum many-body system on a lattice is simulated by a quantum impurity model.



A time consuming step in DMFT simulation is solving for the Green's function of the quantum impurity model.

Image source: http://physics.aalto.fi/en/groups/qd/research/

Bauer et al. suggest speeding up DMFT using quantum computers:

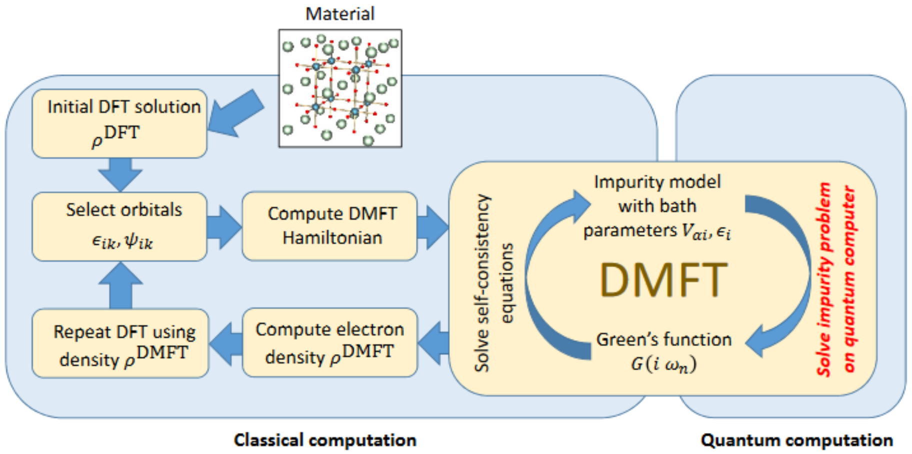


FIG. 1. Overview of the DFT+DMFT approach. In our proposal, the solution of the impurity problem (highlighted in red), which is the computationally limiting step in computations using classical computers, is peformed by a quantum computer.

From Bauer et al. arXiv:1510.03859

Bauer et al. suggest speeding up DMFT using quantum computers:

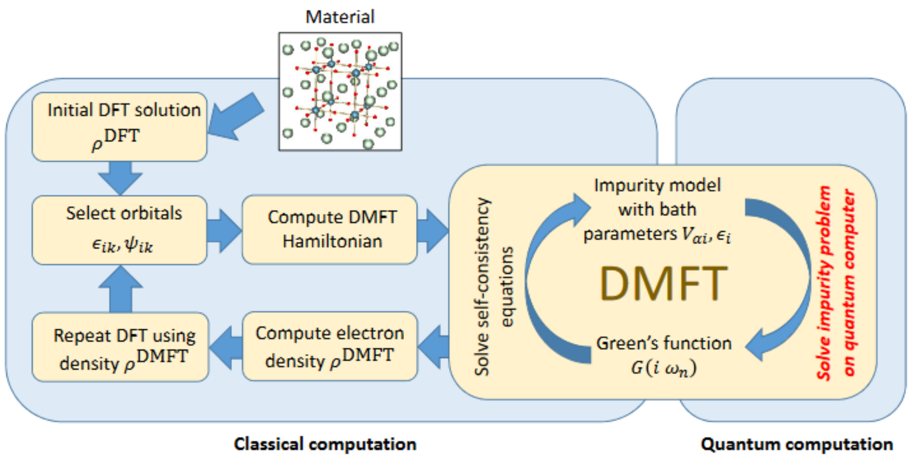


FIG. 1. Overview of the DFT+DMFT approach. In our proposal, the solution of the impurity problem (highlighted in red), which is the computationally limiting step in computations using classical computers, is peformed by a quantum computer.

From Bauer et al.
arXiv:1510.03859

The first step is to prepare the ground state of a quantum impurity model. They propose using quantum adiabatic evolution (efficiency is unknown).

The Green's function is computed by an efficient quantum computation starting from the ground state.

What can we prove about quantum impurity models in the general case?

In this talk we will discuss the computational complexity of approximating the ground energy and computing low energy states…

	n modes (free) Free fermions	m n-m Quantum impurity models	n modes (interacting) Interacting fermions
Concise description of ground state or low energy state?			
Efficient algorithm for ground energy?			

	n modes (free) **Free fermions**	m n-m **Quantum impurity models**	**n modes (interacting)** **Interacting fermions**
Concise description of ground state or low energy state?	✓ Ground state is a Gaussian state, specified by $O(n^2)$ complex numbers.		
Efficient algorithm for ground energy?	✓ $O(n^3)$ algorithm (compute spectrum of a $2n \times 2n$ matrix)		

[Well known]

	n modes (free) Free fermions	m n-m Quantum impurity models	n modes (interacting) Interacting fermions
Concise description of ground state or low energy state?	✓ Ground state is a Gaussian state, specified by $O(n^2)$ complex numbers.		✗ (unless QMA=NP)
Efficient algorithm for ground energy?	✓ $O(n^3)$ algorithm (compute spectrum of a $2n \times 2n$ matrix)		✗ (unless QMA= BPP)
	[Well known]		[Kitaev 2000] [Schuch Verstraete 2007]

	n modes (free) **Free fermions**	m n-m **Quantum impurity models**	n modes (interacting) **Interacting fermions**
Concise description of ground state or low energy state?	✓ Ground state is a Gaussian state, specified by $O(n^2)$ complex numbers.	✓	✗ (unless QMA=NP)
Efficient algorithm for ground energy?	✓ $O(n^3)$ algorithm (compute spectrum of a $2n \times 2n$ matrix)	✓	✗ (unless QMA= BPP)
	[Well known]	**[This talk!]**	[Kitaev 2000] [Schuch Verstraete 2007]

Part I: Setup

Part II: Ground state structure

Part III: Algorithm

Part I: Setup

Part II: Ground state structure

Part III: Algorithm

Fermionic Hilbert space

Hilbert space of n fermionic modes is spanned by Fock basis states

$$|x\rangle = {a_1^\dagger}^{x_1}\ {a_2^\dagger}^{x_2} \ldots {a_n^\dagger}^{x_n} |vac\rangle \qquad\qquad x \in \{0,1\}^n$$

Here $a_j, a_j^\dagger$ are annihilation/creation operators for the jth mode.

Fermionic Hilbert space

Hilbert space of n fermionic modes is spanned by Fock basis states

$$|x\rangle = {a_1^\dagger}^{x_1} \; {a_2^\dagger}^{x_2} \ldots {a_n^\dagger}^{x_n} |vac\rangle \qquad\qquad x \in \{0,1\}^n$$

Here $a_j, a_j^\dagger$ are annihilation/creation operators for the jth mode.

Define **Majorana operators**

$$c_{2j-1} = a_j + a_j^\dagger \qquad\qquad j = 1,2,\ldots,n$$
$$c_{2j} = -i\,(a_j - a_j^\dagger)$$

They are Hermitian and satisfy $c_j c_k + c_k c_j = 2\delta_{jk}$.

Fermionic Hilbert space

Hilbert space of n fermionic modes is spanned by Fock basis states

$$|x\rangle = a_1^{\dagger x_1}\ a_2^{\dagger x_2} \dots a_n^{\dagger x_n} |vac\rangle \qquad\qquad x \in \{0,1\}^n$$

Here $a_j, a_j^\dagger$ are annihilation/creation operators for the jth mode.

Define **Majorana operators**

$$c_{2j-1} = a_j + a_j^\dagger \qquad\qquad j = 1,2,\dots,n$$
$$c_{2j} = -i\,(a_j - a_j^\dagger)$$

They are Hermitian and satisfy $c_j c_k + c_k c_j = 2\delta_{jk}$.

If you prefer qubits…

The Fock basis is naturally represented as the computational basis of n qubits

Majoranas are represented as n-qubit Pauli operators:

$$c_{2j-1} = Z \otimes Z \otimes \cdots Z \otimes X \otimes I_{n-j}$$
$$c_{2j} = \underbrace{Z \otimes Z \otimes \cdots Z}_{j-1} \otimes Y \otimes I_{n-j}$$

Gaussian unitaries and states

A unitary is **Gaussian** if it maps each Majorana to a linear superposition of Majoranas:

$$U c_j U^\dagger = \sum_{k=1}^{2n} R_{jk} c_k$$

Gaussian unitaries and states

A unitary is **Gaussian** if it maps each Majorana to a linear superposition of Majoranas:

$$U c_j U^\dagger = \sum_{k=1}^{2n} R_{jk} c_k \qquad\qquad RR^T = I$$

Gaussian unitaries and states

A unitary is **Gaussian** if it maps each Majorana to a linear superposition of Majoranas:

$$U c_j U^\dagger = \sum_{k=1}^{2n} R_{jk} c_k \qquad RR^T = I$$

A fermionic Gaussian state is of the form $|\phi\rangle = U|0^n\rangle$

Gaussian unitary

Vacuum state

Gaussian unitaries and states

A unitary is **Gaussian** if it maps each Majorana to a linear superposition of Majoranas:

$$U c_j U^\dagger = \sum_{k=1}^{2n} R_{jk} c_k \qquad\qquad RR^T = I$$

A fermionic Gaussian state is of the form $|\phi\rangle = U|0^n\rangle$

Gaussian unitary

Vacuum state

Useful fact #1: Gaussian unitaries diagonalize free fermion Hamiltonians.

Useful fact #2: Gaussian states are fermionic analogues of stabilizer states. We can represent and manipulate them efficiently.

Quantum impurity model Hamiltonian

$$H = H_{bath} + H_{imp}$$

Quantum impurity model Hamiltonian

$$H = H_{bath} + H_{imp}$$

The bath Hamiltonian is a completely general free fermion Hamiltonian

$$H_{bath} = \frac{i}{4} \sum_{i,j=1}^{2n} h_{ij} c_i c_j$$

$h =$ a real antisymmetric matrix

WLOG take $\|h\| \leq 1$

Quantum impurity model Hamiltonian

$$H = H_{bath} + H_{imp}$$

The bath Hamiltonian is a completely general free fermion Hamiltonian

$$H_{bath} = \frac{i}{4}\sum_{i,j=1}^{2n} h_{ij} c_i c_j$$

$h =$ a real antisymmetric matrix

WLOG take $\|h\| \leq 1$

The impurity Hamiltonian acts only on Majoranas $c_1, c_2, \ldots c_m$ but is otherwise unrestricted

$$H_{imp} = \sum_{\substack{x \in \{0,1\}^m \\ |x|\ even}} g_x\, c_1^{x_1} c_2^{x_2} \ldots c_m^{x_m}$$

Since it describes free fermions, $\boldsymbol{H_{bath}}$ is diagonalized by a Gaussian unitary:

$$H_{bath} = E_0 \cdot I + \sum_{j=1}^{n} \epsilon_j \, b_j^\dagger b_j$$

Since it describes free fermions, $\boldsymbol{H_{bath}}$ is diagonalized by a Gaussian unitary:

$$H_{bath} = E_0 \cdot I + \sum_{j=1}^{n} \epsilon_j \, b_j^\dagger b_j$$

Canonical modes: $b_j = U a_j U^\dagger$ for some Gaussian unitary U.

Single-particle excitation energies: $\{\epsilon_j\}$ We have $0 \leq \epsilon_j \leq 1$ because $\|h\| \leq 1$.

Since it describes free fermions, H_{bath} is diagonalized by a Gaussian unitary:

$$H_{bath} = E_0 \cdot I + \sum_{j=1}^{n} \epsilon_j \, b_j^\dagger b_j$$

Canonical modes: $b_j = U a_j U^\dagger$ for some Gaussian unitary U.

Single-particle excitation energies: $\{\epsilon_j\}$ We have $0 \leq \epsilon_j \leq 1$ because $\|h\| \leq 1$.

Bath spectral gap: Write ω for the smallest nonzero ϵ_j.

Since it describes free fermions, H_{bath} is diagonalized by a Gaussian unitary:

WLOG Set to 0 for remainder of talk

$$H_{bath} = E_0 \cdot I + \sum_{j=1}^{n} \epsilon_j \, b_j^\dagger b_j$$

Canonical modes: $b_j = U a_j U^\dagger$ for some Gaussian unitary U.

Single-particle excitation energies: $\{\epsilon_j\}$ We have $0 \le \epsilon_j \le 1$ because $\|h\| \le 1$.

Bath spectral gap: Write ω for the smallest nonzero ϵ_j.

Part I: Setup

Part II: Ground state structure

Part III: Algorithm

Ground state covariance matrix

For any ground state ψ of an impurity model, define an $n \times n$ covariance matrix

$$\boxed{C_{pq} = \langle \psi | b_p^\dagger b_q | \psi \rangle}$$

Ground state covariance matrix

For any ground state ψ of an impurity model, define an $n \times n$ covariance matrix

$$\boxed{C_{pq} = \langle\psi|b_p^\dagger b_q|\psi\rangle}$$

Canonical modes of H_{bath}, i.e.,

$$H_{bath} = \sum_{j=1}^{n} \epsilon_j\, b_j^\dagger b_j$$

Ground state covariance matrix

For any ground state ψ of an impurity model, define an $n \times n$ covariance matrix

$$\boxed{C_{pq} = \langle \psi | b_p^\dagger b_q | \psi \rangle}$$

Ground state covariance matrix

For any ground state ψ of an impurity model, define an $n \times n$ covariance matrix

$$C_{pq} = \langle \psi | b_p^\dagger b_q | \psi \rangle$$

Numerical observation: **Eigenvalues of $\boldsymbol{C}$ decay rapidly**

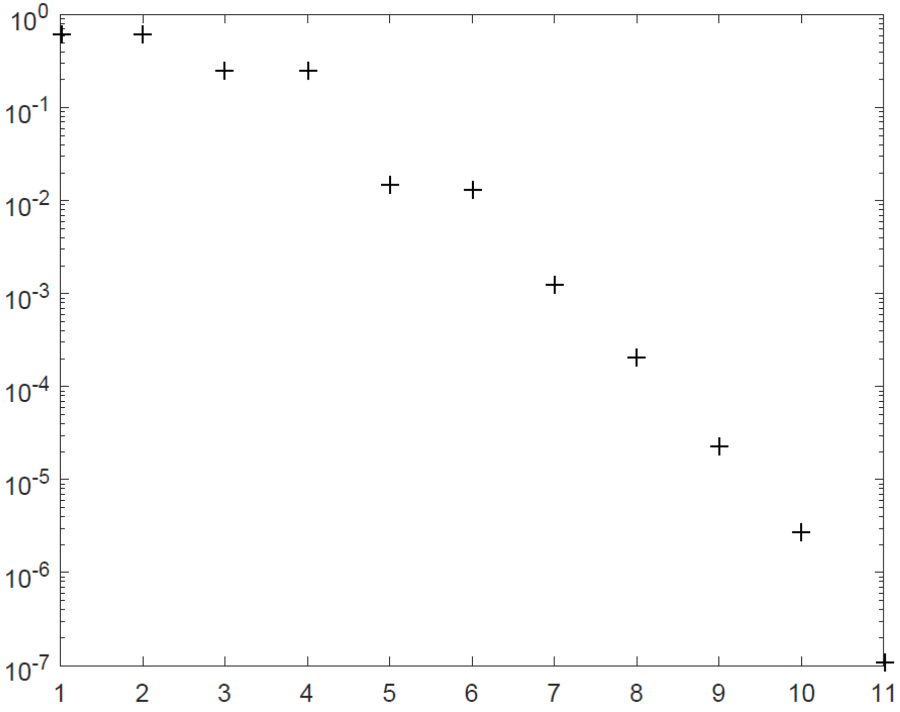
Ground state covariance matrix

For any ground state ψ of an impurity model, define an $n \times n$ covariance matrix

$$C_{pq} = \langle \psi | b_p^\dagger b_q | \psi \rangle$$

Numerical observation: **Eigenvalues of $\boldsymbol{C}$ decay rapidly**

σ_j
(jth eigenvalue)



j

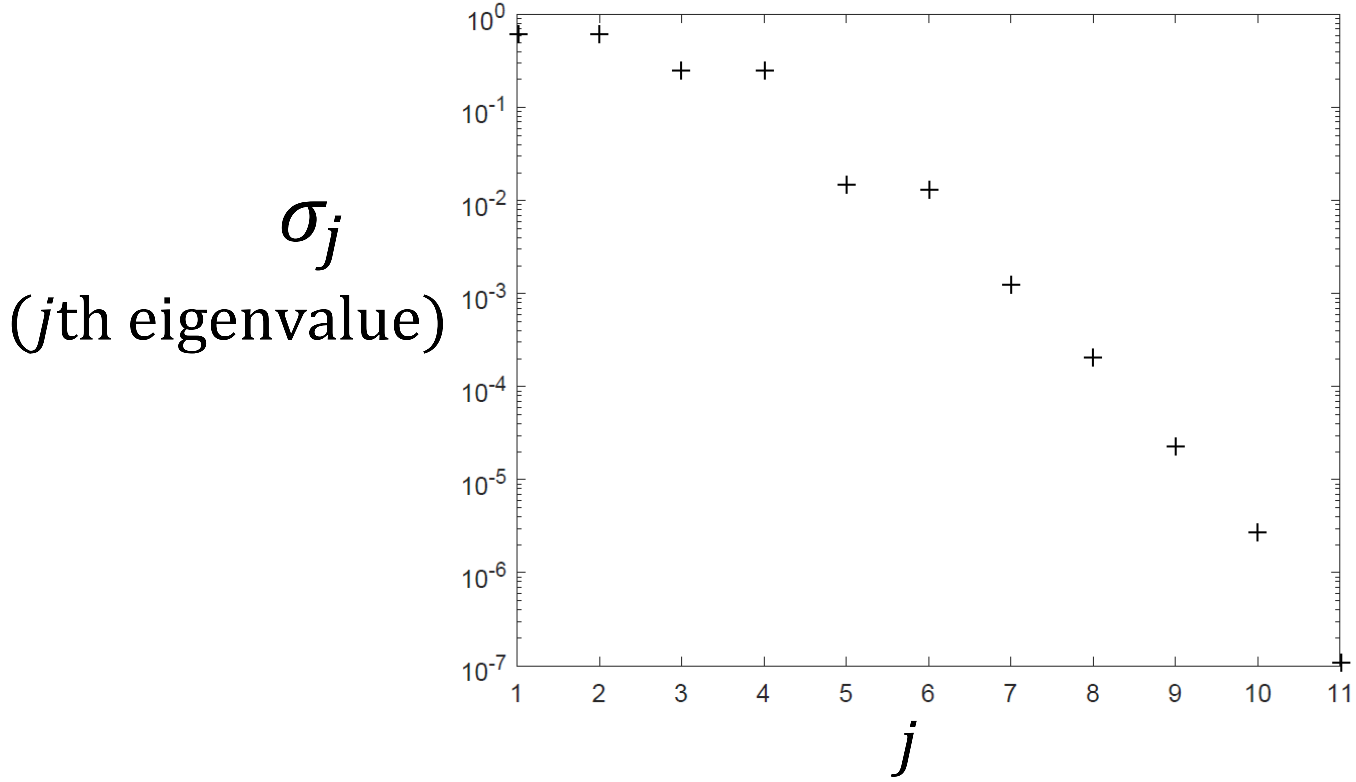
$n = 11$
$m = 4$

Ground state covariance matrix

For any ground state ψ of an impurity model, define an $n \times n$ covariance matrix

$$C_{pq} = \langle \psi | b_p^\dagger b_q | \psi \rangle$$

Numerical observation: **Eigenvalues of C decay rapidly**



$n = 11$
$m = 4$

How general is this?
Why should we care?

Exponential decay theorem

Theorem

There exists a ground state ψ of $H = H_{bath} + H_{imp}$ such that the following holds. Let $\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_n$ be the eigenvalues of the ground state covariance matrix

$$C_{pq} = \langle \psi | b_p^\dagger b_q | \psi \rangle$$

Then

$$\sigma_j \leq const \cdot \exp[-\frac{j}{14m\log(2\omega^{-1})}]$$

Exponential decay theorem

Theorem

There exists a ground state ψ of $H = H_{bath} + H_{imp}$ such that the following holds. Let $\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_n$ be the eigenvalues of the ground state covariance matrix

$$C_{pq} = \langle\psi|b_p^\dagger b_q|\psi\rangle$$

Then

$$\sigma_j \leq const \cdot \exp[-\frac{j}{14m\log(2\omega^{-1})}]$$

Size of impurity

Spectral gap of H_{bath}

Exponential decay theorem

Theorem

There exists a ground state ψ of $H = H_{bath} + H_{imp}$ such that the following holds. Let $\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_n$ be the eigenvalues of the ground state covariance matrix

$$C_{pq} = \langle \psi | b_p^\dagger b_q | \psi \rangle$$

Then

$$\sigma_j \leq const \cdot \exp[-\frac{j}{14m\log(2\omega^{-1})}]$$

Exponential decay theorem

Theorem

There exists a ground state ψ of $H = H_{bath} + H_{imp}$ such that the following holds. Let $\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_n$ be the eigenvalues of the ground state covariance matrix

$$C_{pq} = \langle \psi | b_p^\dagger b_q | \psi \rangle$$

Then

$$\sigma_j \leq const \cdot \exp[-\frac{j}{14m\log(2\omega^{-1})}]$$

The proof has two steps:

1. Using a variational characterization of ground states we show that C satisfies a set of matrix inequalities

$0 \leq C \leq I$	$\Lambda^2 = \Lambda$	$\omega I \leq E \leq I$
$rank(\Lambda) \geq n - m$	$\Lambda C E \Lambda \leq 0$	$\Lambda[C, E]\Lambda = 0$

Exponential decay theorem

Theorem

There exists a ground state ψ of $H = H_{bath} + H_{imp}$ such that the following holds. Let $\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_n$ be the eigenvalues of the ground state covariance matrix

$$C_{pq} = \langle \psi | b_p^\dagger b_q | \psi \rangle$$

Then

$$\sigma_j \leq const \cdot \exp[-\frac{j}{14m\log(2\omega^{-1})}]$$

The proof has two steps:

1. Using a variational characterization of ground states we show that C satisfies a set of matrix inequalities

$0 \leq C \leq I$	$\Lambda^2 = \Lambda$	$\omega I \leq E \leq I$
$rank(\Lambda) \geq n - m$	$\Lambda C E \Lambda \leq 0$	$\Lambda[C, E]\Lambda = 0$

2. We show that any C satisfying the matrix inequalities has the claimed exponential decay. This part uses Zolotarev's rational approximation to the square root function.

Exponential decay theorem

Theorem
There exists a ground state ψ of $H = H_{bath} + H_{imp}$ such that the following holds. Let $\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_n$ be the eigenvalues of the ground state covariance matrix

$$C_{pq} = \langle \psi | b_p^\dagger b_q | \psi \rangle$$

Then

$$\sigma_j \leq const \cdot \exp[-\frac{j}{14m\log(2\omega^{-1})}]$$

Size of impurity

Spectral gap of H_{bath}

The theorem holds for all impurity models and has no dependence on H_{imp}.

Exponential decay theorem

Theorem

There exists a ground state ψ of $H = H_{bath} + H_{imp}$ such that the following holds. Let $\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_n$ be the eigenvalues of the ground state covariance matrix

$$C_{pq} = \langle\psi|b_p^\dagger b_q|\psi\rangle$$

Then

$$\sigma_j \leq const \cdot \exp[-\frac{j}{14m\log(2\omega^{-1})}]$$

Size of impurity

Spectral gap of H_{bath}

The theorem holds for all impurity models and has no dependence on $\boldsymbol{H_{imp}}$.

A slightly stronger version holds if the bath does not have zero energy excitations.

Exponential decay theorem

Theorem

There exists a ground state ψ of $H = H_{bath} + H_{imp}$ such that the following holds. Let $\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_n$ be the eigenvalues of the ground state covariance matrix

$$C_{pq} = \langle\psi|b_p^\dagger b_q|\psi\rangle$$

Then

$$\sigma_j \leq const \cdot \exp[-\frac{j}{14m\log(2\omega^{-1})}]$$

Size of impurity

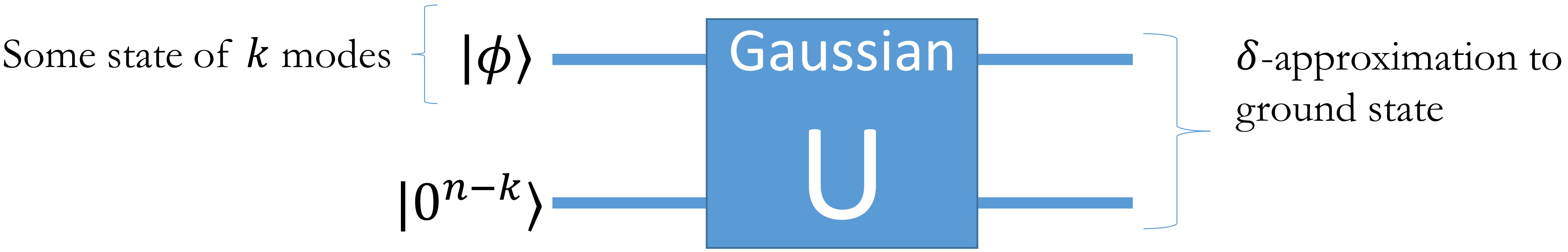
Spectral gap of H_{bath}

The theorem holds for all impurity models and has no dependence on $\boldsymbol{H_{imp}}$.

A slightly stronger version holds if the bath does not have zero energy excitations.

An important corollary is that a ground state has a concise classical representation…

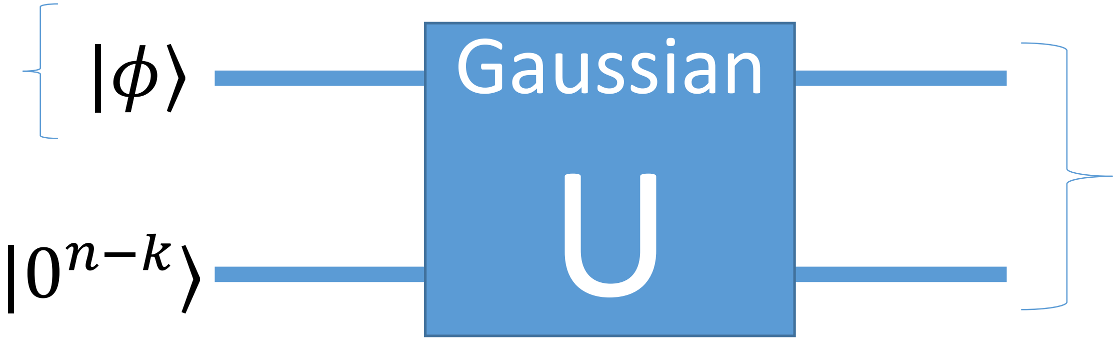
Concise representation of ground state



Can we make this work with small *k*?

Concise representation of ground state

Some state of k modes



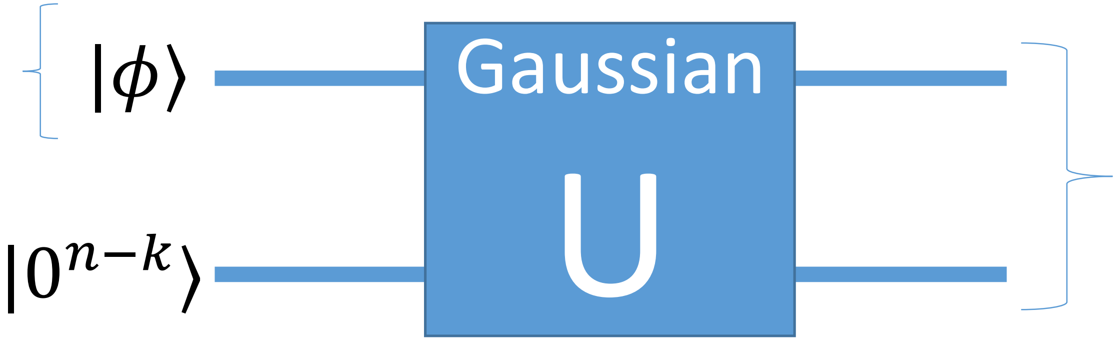
δ-approximation to ground state

A superposition of 2^k Gaussian states

Can we make this work with small *k*?

Concise representation of ground state

Some state of k modes



δ-approximation to ground state

A superposition of 2^k Gaussian states

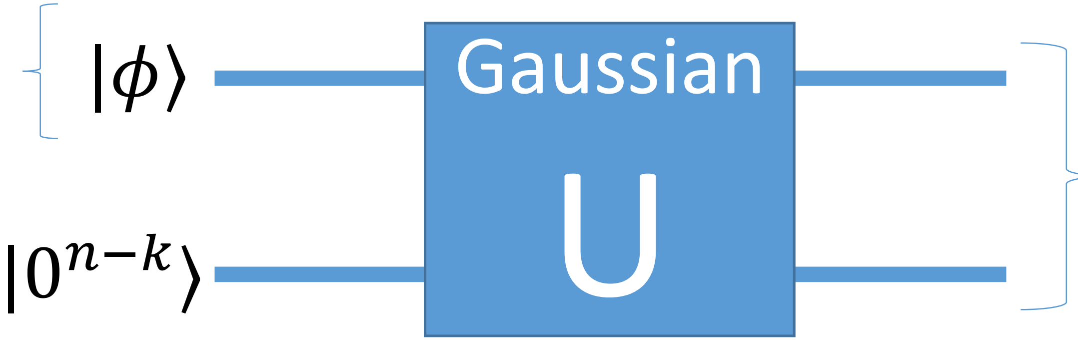
Corollary of Exponential Decay Theorem

It suffices to take

$$k = O(1) \cdot m \log 2\omega^{-1} \cdot [\log \delta^{-1} + \log m + \log\log 2\omega^{-1}]$$

Concise representation of ground state

Some state of k modes



δ-approximation to ground state

A superposition of 2^k Gaussian states

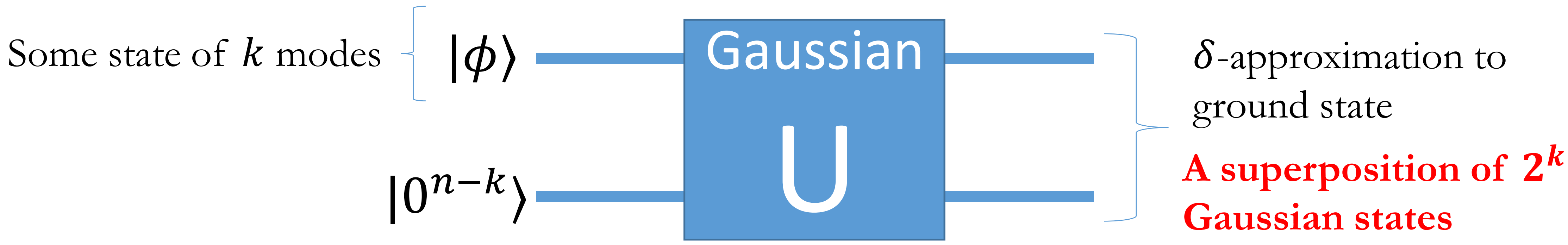
Corollary of Exponential Decay Theorem

It suffices to take

$$k = O(1) \cdot m \log 2\omega^{-1} \cdot [\log \delta^{-1} + \log m + \log\log 2\omega^{-1}]$$

The "Gaussian rank" $\chi = 2^k$ of the ground state approximation has no explicit dependence on n !

Concise representation of ground state



Corollary of Exponential Decay Theorem

It suffices to take

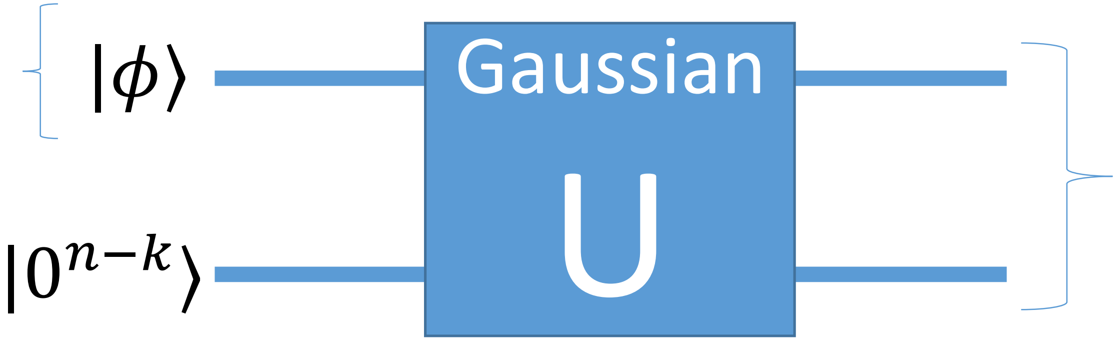
$$k = O(1) \cdot m \log 2\omega^{-1} \cdot [\log \delta^{-1} + \log m + \log \log 2\omega^{-1}]$$

The "Gaussian rank" $\chi = 2^k$ of the ground state approximation has no explicit dependence on n !

All excitations are localized on k modes by a Gaussian unitary.

Concise representation of ground state

Some state of k modes



δ-approximation to ground state

A superposition of 2^k Gaussian states

Corollary of Exponential Decay Theorem

It suffices to take

$$k = O(1) \cdot m \log 2\omega^{-1} \cdot [\log \delta^{-1} + \log m + \log\log 2\omega^{-1}]$$

The "Gaussian rank" $\chi = 2^k$ of the ground state approximation has no explicit dependence on n !

All excitations are localized on k modes by a Gaussian unitary.

(we can prove a slightly stronger bound $\chi = poly(\omega^{-1})$ using an approximation without this property…)

Concise representation of ground state

Corollary of Exponential Decay Theorem

It suffices to take

$$k = O(1) \cdot m \log 2\omega^{-1} \cdot [\log \delta^{-1} + \log m + \log\log 2\omega^{-1}]$$

Proof idea:

Almost all eigenvalues of the ground state covariance matrix C are tiny (exponential decay theorem)

Concise representation of ground state

Corollary of Exponential Decay Theorem

It suffices to take
$$k = O(1) \cdot m \log 2\omega^{-1} \cdot [\log \delta^{-1} + \log m + \log\log 2\omega^{-1}]$$

Proof idea:

Almost all eigenvalues of the ground state covariance matrix C are tiny (exponential decay theorem)

Suppose $C\vec{v} \approx 0$. Then a new fermi mode operator $B = \sum_{j=1}^{n} v_j b_j$ satisfies $\langle\psi|B^\dagger B|\psi\rangle \approx 0.$

Concise representation of ground state

Corollary of Exponential Decay Theorem

It suffices to take
$$k = O(1) \cdot m \log 2\omega^{-1} \cdot [\log \delta^{-1} + \log m + \log\log 2\omega^{-1}]$$

Proof idea:

Almost all eigenvalues of the ground state covariance matrix C are tiny (exponential decay theorem)

Suppose $C\vec{v} \approx 0$. Then a new fermi mode operator $B = \sum_{j=1}^{n} v_j b_j$ satisfies $\langle\psi|B^\dagger B|\psi\rangle \approx 0$.

So for each tiny eigenvalue of C we have a fermi mode which is unoccupied with high probability.

Choose a Gaussian unitary which transforms to this new set of fermi modes.

	Quantum impurity models
Concise description of ground state or low energy state?	✓ **Answer #1:** A ground state ψ is approximated to any constant precision by a superposition of $poly(\omega^{-1})$ Gaussian states.
Efficient algorithm for ground energy?	

	Quantum impurity models
Concise description of ground state or low energy state?	✓ **Answer #1:** A ground state ψ is approximated to any constant precision by a superposition of $poly(\omega^{-1})$ Gaussian states.
Efficient algorithm for ground energy?	The results discussed so far are not algorithmic.

Part I: Setup

Part II: Ground state structure

Part III: Algorithm

Algorithm

Theorem

There is a classical algorithm which computes the ground energy of a quantum impurity model to within a given error tolerance ϵ. The runtime of the algorithm is

$$n^3 \exp[O(m \log^3(m\epsilon^{-1}))]$$

Algorithm

Theorem

There is a classical algorithm which computes the ground energy of a quantum impurity model to within a given error tolerance ϵ. The runtime of the algorithm is

$$n^3 \exp[O(m \log^3(m\epsilon^{-1}))]$$

Runtime scales polynomially in n and quasipolynomially in the inverse error ϵ^{-1}.

Algorithm

Theorem
There is a classical algorithm which computes the ground energy of a quantum impurity model to within a given error tolerance ϵ. The runtime of the algorithm is

$$n^3 \exp[O(m \log^3(m\epsilon^{-1}))]$$

Runtime scales polynomially in n and quasipolynomially in the inverse error ϵ^{-1}.

Scaling with m is close to optimal.

Algorithm

Theorem
There is a classical algorithm which computes the ground energy of a quantum impurity model to within a given error tolerance ϵ. The runtime of the algorithm is

$$n^3 \exp[O(m \log^3(m\epsilon^{-1}))]$$

Runtime scales polynomially in n and quasipolynomially in the inverse error ϵ^{-1}.

Scaling with m is close to optimal.

The algorithm produces a classical description of a state with energy at most ϵ. This state is a superposition of χ Gaussian states, with

$$\chi = \exp[O(m \log^3(m\epsilon^{-1}))]$$

The algorithm uses the following two facts…

“Decoupling trick” **[useful if $\boldsymbol{H_{bath}}$ is highly degenerate. Proof is elementary linear algebra]**

If the bath Hamiltonian has D distinct single-particle energies then we apply a Gaussian unitary transformation which decouples all except Dm modes from the impurity.

The algorithm uses the following two facts…

"Decoupling trick" **[useful if H_{bath} is highly degenerate. Proof is elementary linear algebra]**
If the bath Hamiltonian has D distinct single-particle energies then we apply a Gaussian unitary transformation which decouples all except Dm modes from the impurity.

"Few excitation subspace": **[Consequence of exponential decay theorem]**
To approximate ground energy with precision ϵ we can restrict our attention to the subspace with at most $O\left(m log^2(m\epsilon^{-1})\right)$ bath excitations.

Algorithm outline

Step 1: Diagonalize the free fermion Hamiltonian $\boldsymbol{H_{bath}}$

$$H_{bath} = \sum_{j=1}^{n} \epsilon_j \, b_j^\dagger b_j$$

Computing all canonical modes and excitation energies takes time $O(n^3)$ using linear algebra.

Algorithm outline

Step 2: **Discretize single-particle energies of $\boldsymbol{H_{bath}}$ to a uniform grid with spacing $\boldsymbol{\Delta}$.**

Original impurity problem

$$H_{bath} = \sum_{j=1}^{n} \epsilon_j \, b_j^\dagger b_j \qquad 0 \le \epsilon_j \le 1$$

$$H = H_{bath} + H_{imp}$$

Discretized impurity problem

$$\widetilde{H}_{bath} = \sum_{j=1}^{n} E_j \, b_j^\dagger b_j \qquad \epsilon_j \le E_j \le \epsilon_j + \Delta$$

$$\widetilde{H} = \widetilde{H}_{bath} + H_{imp}$$

Algorithm outline

Step 2: Discretize single-particle energies of $\boldsymbol{H_{bath}}$ to a uniform grid with spacing $\boldsymbol{\Delta}$.

Original impurity problem

$$H_{bath} = \sum_{j=1}^{n} \epsilon_j \, b_j^\dagger b_j \qquad 0 \le \epsilon_j \le 1$$

$$H = H_{bath} + H_{imp}$$

Discretized impurity problem

$$\widetilde{H}_{bath} = \sum_{j=1}^{n} E_j \, b_j^\dagger b_j \qquad \epsilon_j \le E_j \le \epsilon_j + \Delta$$

$$\widetilde{H} = \widetilde{H}_{bath} + H_{imp}$$

We want the error introduced by the discretization to be $\boldsymbol{O(\epsilon)}$. How fine should we choose the grid spacing $\boldsymbol{\Delta}$?

Algorithm outline

Step 2: Discretize single-particle energies of $\boldsymbol{H_{bath}}$ to a uniform grid with spacing $\boldsymbol{\Delta}$.

Original impurity problem

$$H_{bath} = \sum_{j=1}^{n} \epsilon_j \, b_j^\dagger b_j \qquad 0 \leq \epsilon_j \leq 1$$

$$H = H_{bath} + H_{imp}$$

Discretized impurity problem

$$\widetilde{H}_{bath} = \sum_{j=1}^{n} E_j \, b_j^\dagger b_j \qquad \epsilon_j \leq E_j \leq \epsilon_j + \Delta$$

$$\widetilde{H} = \widetilde{H}_{bath} + H_{imp}$$

We want the error introduced by the discretization to be $\boldsymbol{O(\epsilon)}$. How fine should we choose the grid spacing $\boldsymbol{\Delta}$?

Amazing fact:

It suffices to choose $\Delta = \dfrac{\epsilon}{m log^2(m\epsilon^{-1})}$

Algorithm outline

Step 2: **Discretize single-particle energies of $\boldsymbol{H_{bath}}$ to a uniform grid with spacing $\boldsymbol{\Delta}$.**

Original impurity problem

$$H_{bath} = \sum_{j=1}^{n} \epsilon_j \, b_j^\dagger b_j \qquad 0 \le \epsilon_j \le 1$$

$$H = H_{bath} + H_{imp}$$

Discretized impurity problem

$$\widetilde{H}_{bath} = \sum_{j=1}^{n} E_j \, b_j^\dagger b_j \qquad \epsilon_j \le E_j \le \epsilon_j + \Delta$$

$$\widetilde{H} = \widetilde{H}_{bath} + H_{imp}$$

We want the error introduced by the discretization to be $\boldsymbol{O(\epsilon)}$. How fine should we choose the grid spacing $\boldsymbol{\Delta}$?

Amazing fact:
It suffices to choose $\Delta = \dfrac{\epsilon}{m \log^2(m\epsilon^{-1})}$

This seems too coarse (doesn't depend on $\boldsymbol{n}$)! The norm $\|\boldsymbol{H} - \widetilde{\boldsymbol{H}}\|$ can be large!

Algorithm outline

Step 2: **Discretize single-particle energies of $\boldsymbol{H_{bath}}$ to a uniform grid with spacing $\boldsymbol{\Delta}$.**

Original impurity problem

$$H_{bath} = \sum_{j=1}^{n} \epsilon_j \, b_j^\dagger b_j \qquad 0 \le \epsilon_j \le 1$$

$$H = H_{bath} + H_{imp}$$

Discretized impurity problem

$$\widetilde{H}_{bath} = \sum_{j=1}^{n} E_j \, b_j^\dagger b_j \qquad \epsilon_j \le E_j \le \epsilon_j + \Delta$$

$$\widetilde{H} = \widetilde{H}_{bath} + H_{imp}$$

We want the error introduced by the discretization to be $\boldsymbol{O(\epsilon)}$. How fine should we choose the grid spacing $\boldsymbol{\Delta}$?

Amazing fact:
It suffices to choose $\Delta = \dfrac{\epsilon}{m\log^2(m\epsilon^{-1})}$

This seems too coarse (doesn't depend on $\boldsymbol{n}$)! The norm $\|\boldsymbol{H - \widetilde{H}}\|$ can be large!

It works because $\boldsymbol{H - \widetilde{H}}$ has norm $\boldsymbol{O(\epsilon)}$ <u>when restricted to the few excitation subspace</u>.

Algorithm outline

Because the grid is very coarse, the discretized bath Hamiltonian is highly degenerate.

The number of distinct single particle energies is at most $\frac{1}{\Delta} = m\epsilon^{-1} log^2(m\epsilon^{-1})$

Algorithm outline

Because the grid is very coarse, the discretized bath Hamiltonian is highly degenerate.

The number of distinct single particle energies is at most $\frac{1}{\Delta} = m\epsilon^{-1} log^2(m\epsilon^{-1})$

Use decoupling trick! This decouples almost all modes from the impurity by a Gaussian unitary.

Number of modes left coupled to the impurity: $\boxed{N_{modes} \leq \frac{m}{\Delta} = m^2\epsilon^{-1} log^2(m\epsilon^{-1})}$

Algorithm outline

Because the grid is very coarse, the discretized bath Hamiltonian is highly degenerate.

The number of distinct single particle energies is at most $\dfrac{1}{\Delta} = m\epsilon^{-1}log^2(m\epsilon^{-1})$

Use decoupling trick! This decouples almost all modes from the impurity by a Gaussian unitary.

Number of modes left coupled to the impurity: $\boxed{N_{modes} \leq \dfrac{m}{\Delta} = m^2\epsilon^{-1}log^2(m\epsilon^{-1})}$

We can restrict to few excitation subspace: $\boxed{N_{excitations} \leq m log^2(m\epsilon^{-1})}$

Algorithm outline

Because the grid is very coarse, the discretized bath Hamiltonian is highly degenerate.

The number of distinct single particle energies is at most $\frac{1}{\Delta} = m\epsilon^{-1}log^2(m\epsilon^{-1})$

Use decoupling trick! This decouples almost all modes from the impurity by a Gaussian unitary.

Number of modes left coupled to the impurity: $\boxed{N_{modes} \leq \frac{m}{\Delta} = m^2\epsilon^{-1}log^2(m\epsilon^{-1})}$

We can restrict to few excitation subspace: $\boxed{N_{excitations} \leq mlog^2(m\epsilon^{-1})}$

Final step of algorithm: compute the smallest eigenvalue of H in a subspace of dimension at most

$$\sum_{j=0}^{N_{excitations}} \binom{N_{modes}}{j} = \exp[O(m\log^3(m\epsilon^{-1}))]$$

	Quantum impurity models
Concise description of ground state or low energy state?	✓ **Answer #1:** A ground state ψ is approximated to any constant precision by a superposition of $poly(\omega^{-1})$ Gaussian states.
Efficient algorithm for ground energy?	✓ Classical algorithm with runtime: $n^3 \exp[O(m \log^3(m\epsilon^{-1}))]$

	Quantum impurity models
Concise description of ground state or low energy state?	✓ **Answer #1:** A ground state ψ is approximated to any constant precision by a superposition of $poly(\omega^{-1})$ Gaussian states. **Answer #2:** For any ϵ there exists a state with energy $\leq \epsilon$ and Gaussian rank $\chi = exp[O(m\, log^3(m\epsilon^{-1}))]$.
Efficient algorithm for ground energy?	✓ Classical algorithm with runtime: $n^3 \exp[O(m \log^3(m\epsilon^{-1}))]$

Extensions and open questions

Can the quasipolynomial scaling with ϵ be improved?

What is the complexity of approximating the ground energy with precision $\epsilon = poly(n)^{-1}$?

We prove that (a decision version of) this problem is contained in the complexity class QCMA.

Extensions and open questions

Can the quasipolynomial scaling with ϵ be improved?
What is the complexity of approximating the ground energy with precision $\epsilon = poly(n)^{-1}$?
We prove that (a decision version of) this problem is contained in the complexity class QCMA.

Is the algorithm practical?
We give a simplified algorithm based on using the set of low rank Gaussian states as a variational ansatz.

Extensions and open questions

Can the quasipolynomial scaling with ϵ be improved?
What is the complexity of approximating the ground energy with precision $\epsilon = poly(n)^{-1}$?
We prove that (a decision version of) this problem is contained in the complexity class QCMA.

Is the algorithm practical?
We give a simplified algorithm based on using the set of low rank Gaussian states as a variational ansatz.

What about the complexity of simulating the time evolution of quantum impurity models?
A result of Brod and Childs establishes that evolution with a time-dependent impurity model Hamiltonian cannot be efficiently simulated on a classical computer (unless BPP=BQP).

Extensions and open questions

Can the quasipolynomial scaling with ϵ be improved?
What is the complexity of approximating the ground energy with precision $\epsilon = poly(n)^{-1}$?
We prove that (a decision version of) this problem is contained in the complexity class QCMA.

Is the algorithm practical?
We give a simplified algorithm based on using the set of low rank Gaussian states as a variational ansatz.

What about the complexity of simulating the time evolution of quantum impurity models?
A result of Brod and Childs establishes that evolution with a time-dependent impurity model Hamiltonian cannot be efficiently simulated on a classical computer (unless BPP=BQP).

Further applications of low rank Gaussian states? Analogs between Gaussian/stabilizer states?
We provide some new technical tools in this direction. For example, a condition under which an ensemble of Gaussian states forms an analog of a 2-design.

Thanks!