Complexity of quantum impurity problems

Sergey Bravyi

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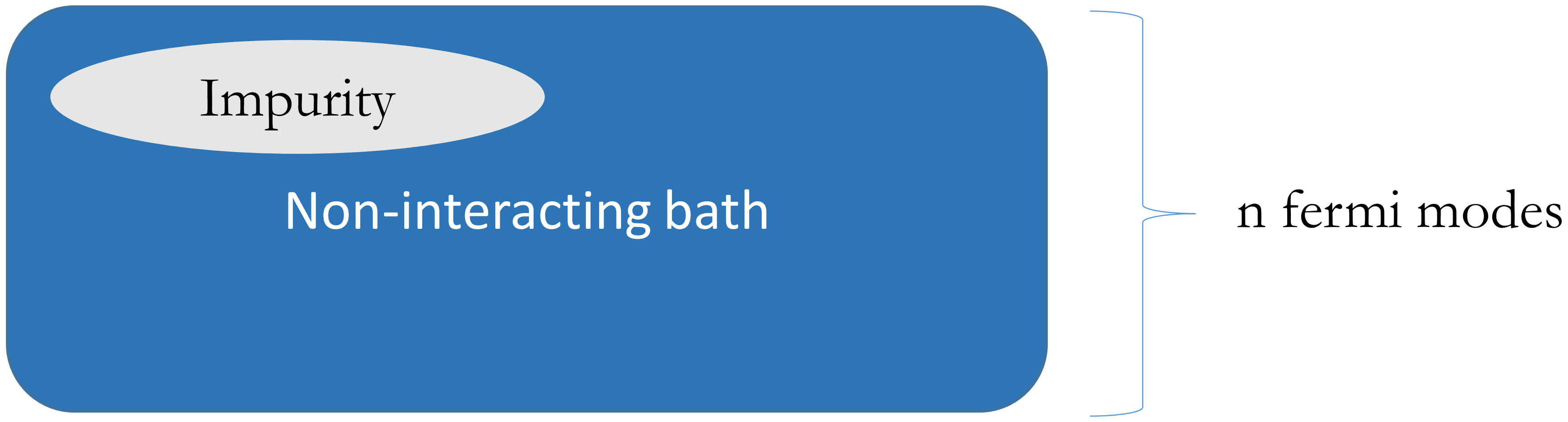
arXiv:1609.00735

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



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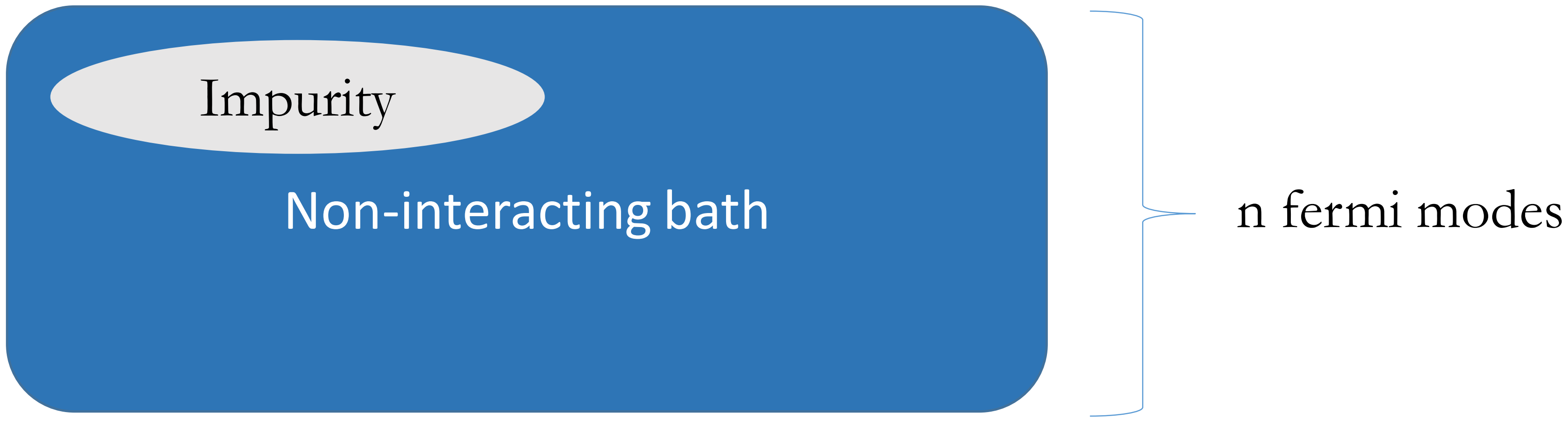


$$H = H_{bath} + H_{imp}$$

Non-interacting (quadratic)

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

Quantum impurity models were introduced to study the Kondo effect:

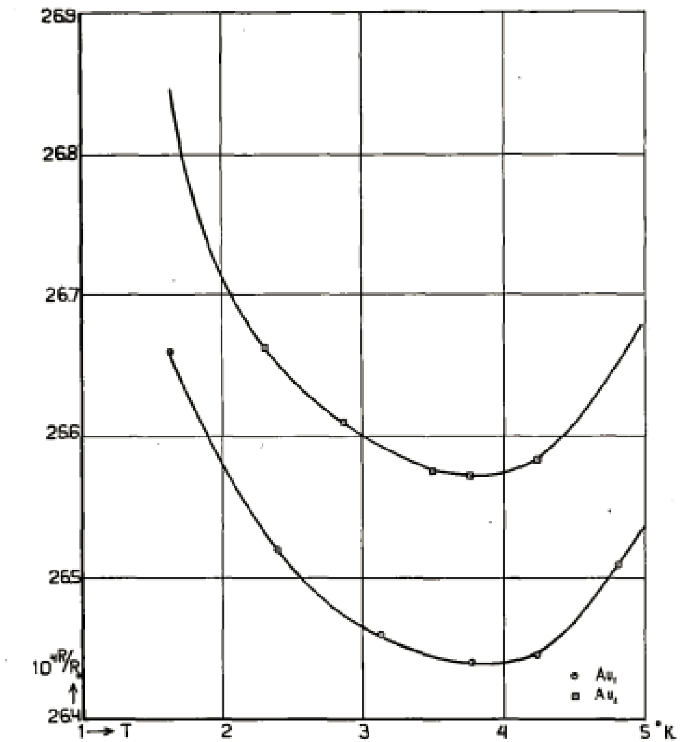


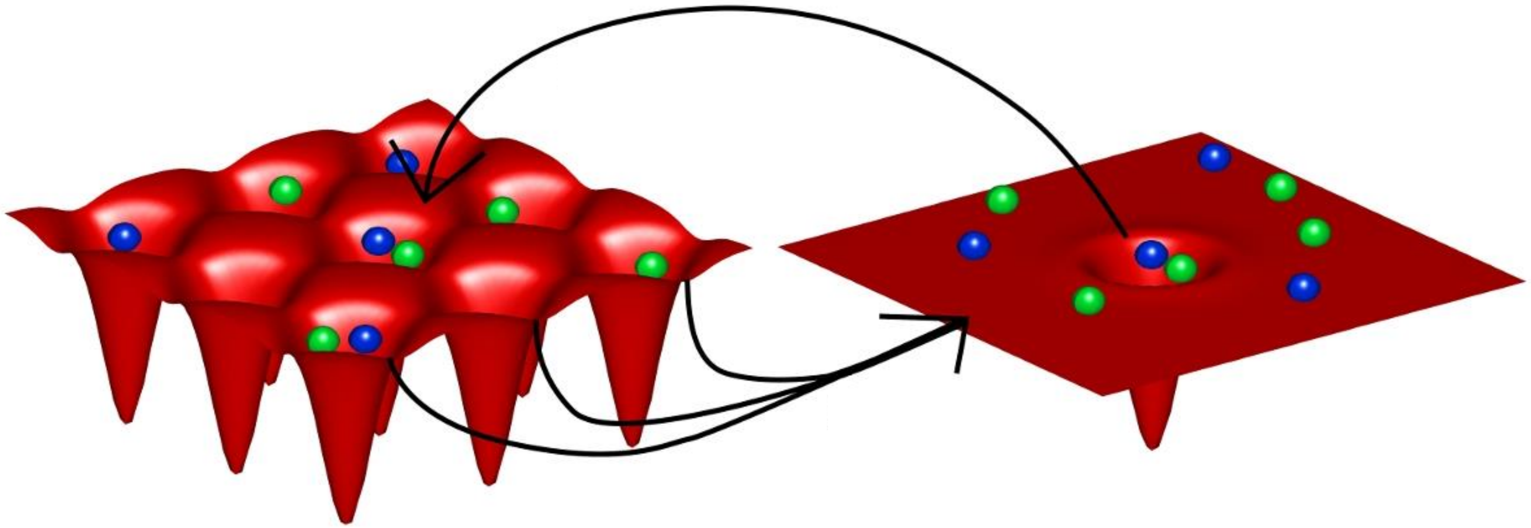
Fig. 1. Resistance of *Au* between 1°K. and 5°K.

"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:

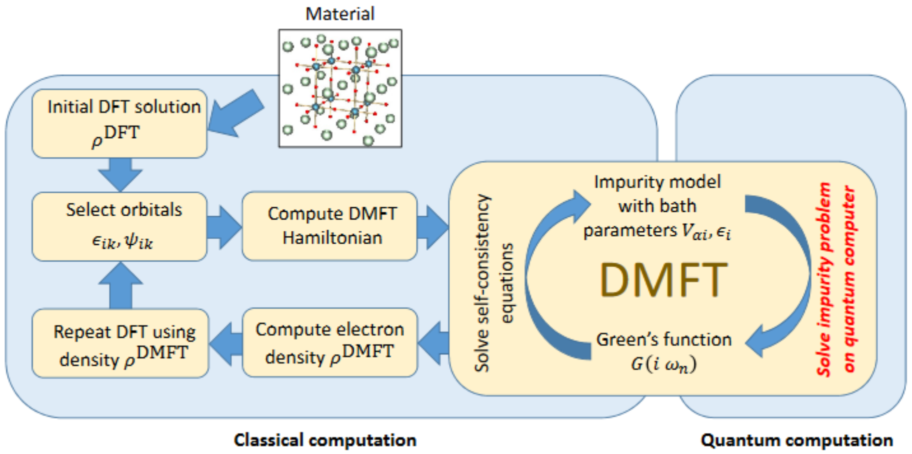


FIG. 1. Overview of the DFT+DMFT approach. In our proposal, the solution of the impurity problem (highlighted in red), which is the computationally limiting step in computations using classical computers, is peformed by a quantum computer.

From Bauer et al. arXiv:1510.03859

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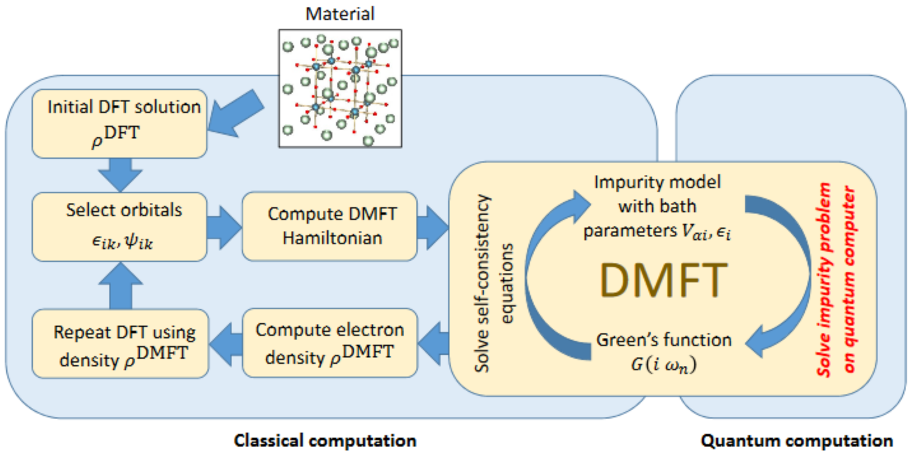

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The first step is to prepare the ground state of a quantum impurity model. They propose using quantum adiabatic evolution (efficiency is unknown).

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?			

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Efficient algorithm for ground energy?	✓ $O(n^3)$ algorithm (compute spectrum of a $2n \times 2n$ matrix)		

[Well known]

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	[Well known]		[Kitaev 2000] [Schuch Verstraete 2007]

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	[Well known]	**[This talk!]**	[Kitaev 2000] [Schuch Verstraete 2007]

Part I: Setup

Part II: Ground state structure

Part III: Algorithm

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Fermionic Hilbert space

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

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

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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 $c_j c_k + c_k c_j = 2\delta_{jk}$.

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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:

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

Gaussian unitaries and states

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

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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

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

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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 $\|h\| \leq 1$

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

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

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

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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

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▶ **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

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

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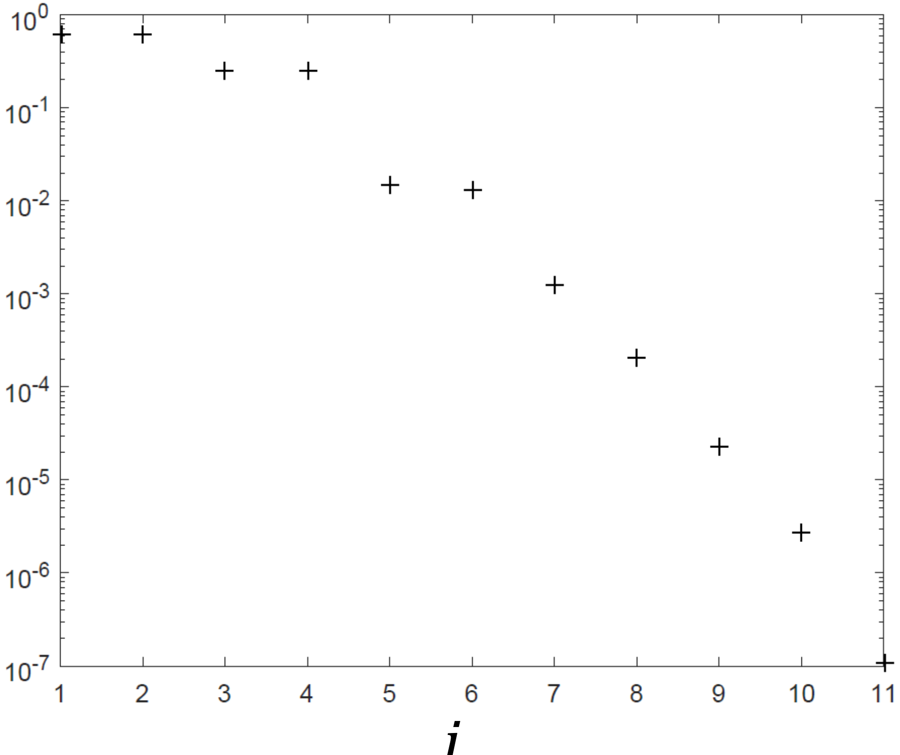
σ_j
(jth eigenvalue)



$n = 11$
$m = 4$

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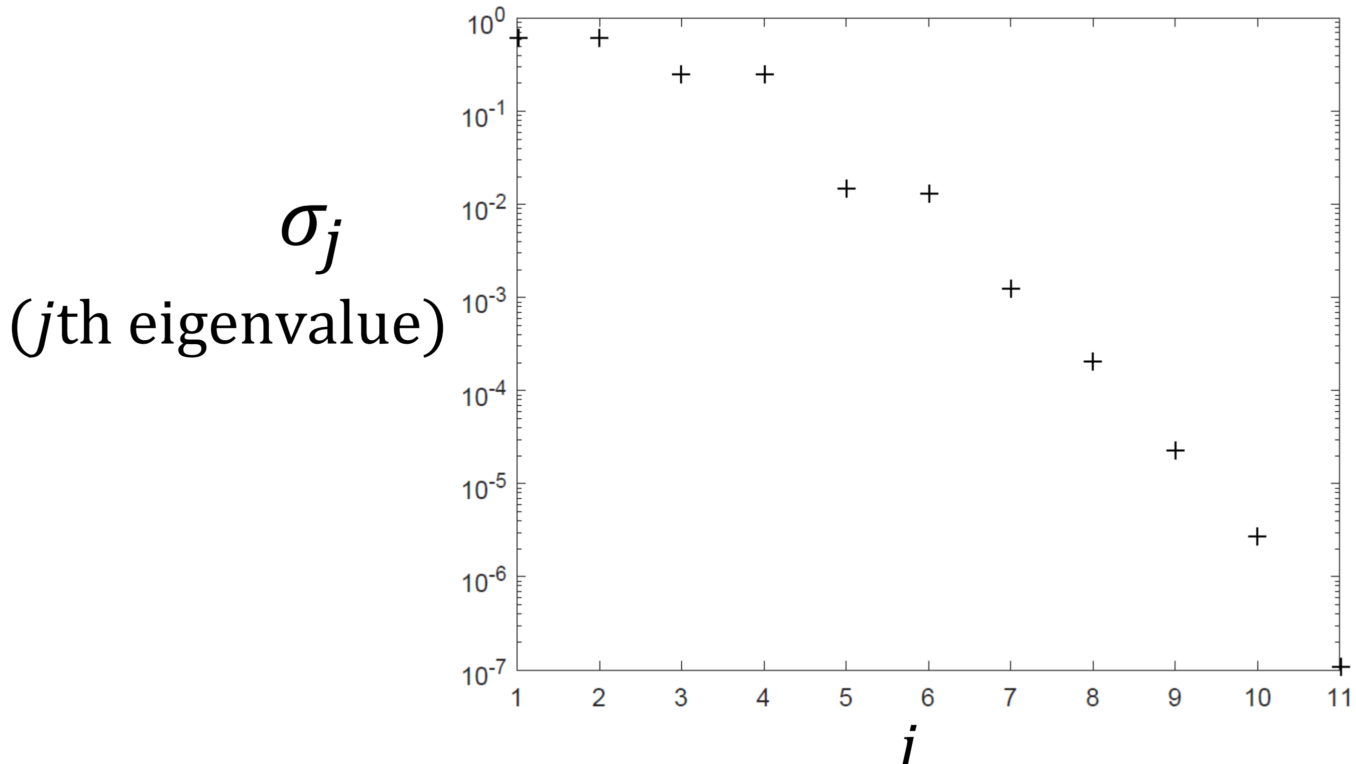

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How general is this?
Why should we care?

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

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Then

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The proof has two steps:

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

$0 \leq C \leq I$	$\Lambda^2 = \Lambda$	$\omega I \leq E \leq I$
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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.

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Size of impurity (→ m)

Spectral gap of H_{bath} (→ ω)

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

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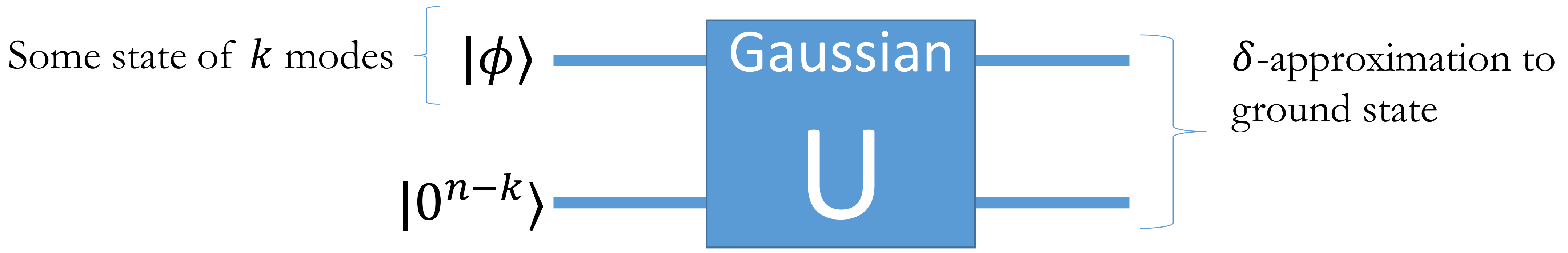
An important corollary is that a ground state has a concise classical representation…

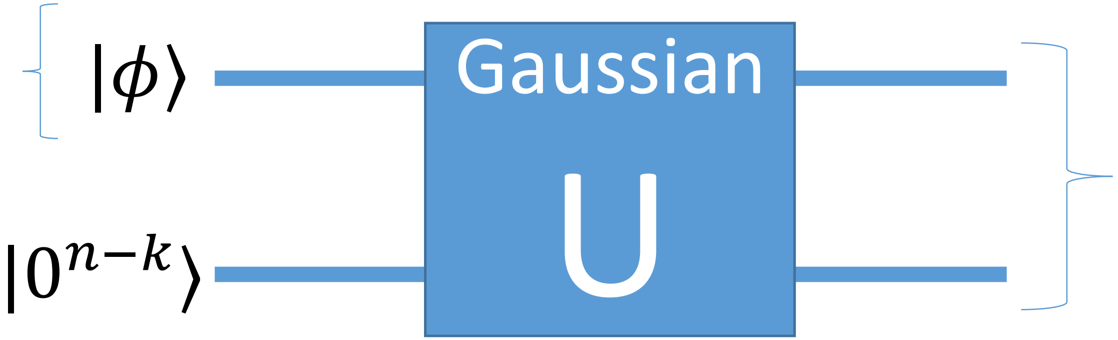
Concise representation of ground state



Can we make this work with small *k*?

Concise representation of ground state

Some state of k modes



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A superposition of 2^k Gaussian states

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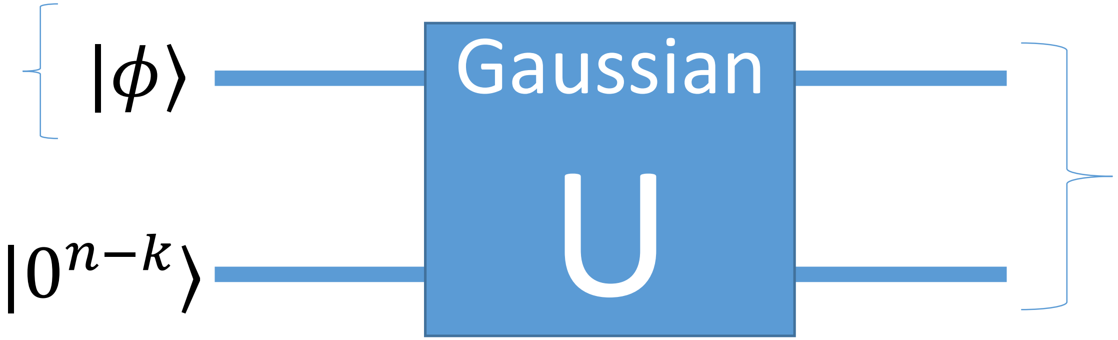

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It suffices to take

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

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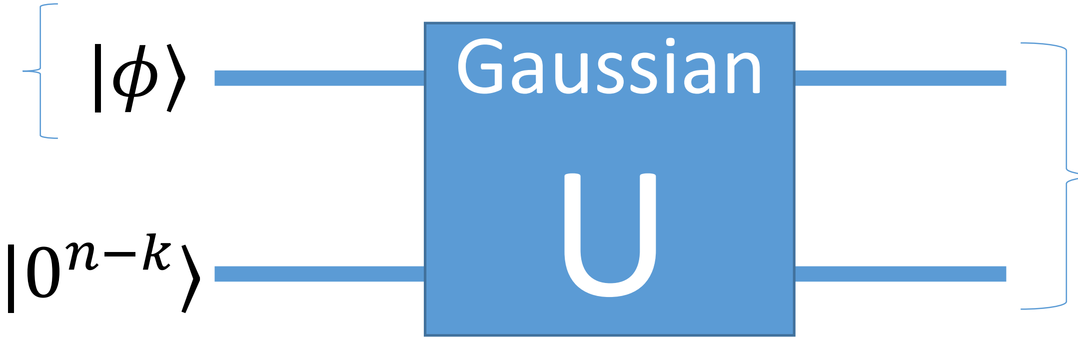

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(we can prove a slightly stronger bound $\chi = poly(\omega^{-1})$ using an approximation without this property…)

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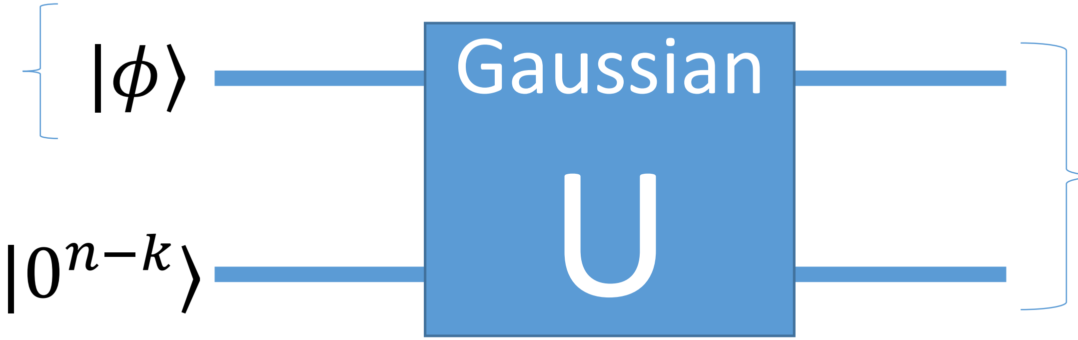

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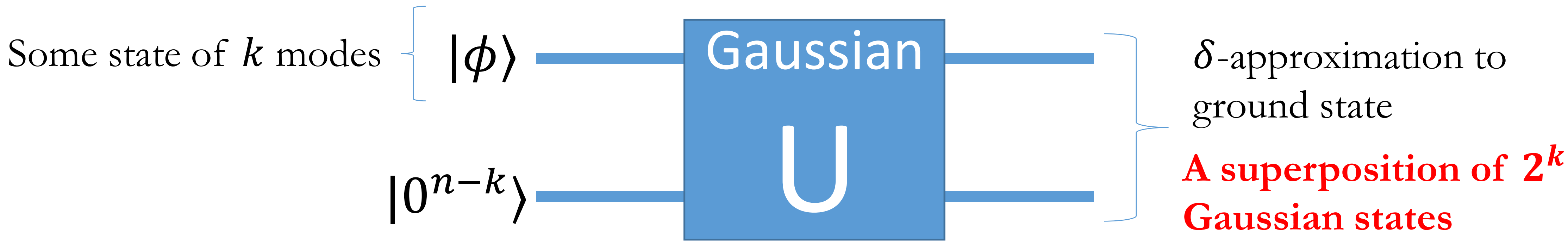

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Suppose $C\vec{v} \approx 0$. Then a new fermi mode operator $B = \sum_{j=1}^{n} v_j b_j$ satisfies $\langle\psi|B^\dagger B|\psi\rangle \approx 0.$

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.
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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.

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▶ **Part III: Algorithm**

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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 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.

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“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

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

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

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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.
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	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.

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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!