Complexity of Quantum Impurity Problems

Sergey Bravyi, David Gosset

IBM T.J. Watson Research Center, Yorktown Heights, NY, USA. E-mail: sbravyi@us.ibm.com; dngosset@us.ibm.com

Received: 28 November 2016 / Accepted: 6 June 2017
Published online: 31 August 2017 – © Springer-Verlag GmbH Germany 2017

Abstract: We give a quasi-polynomial time classical algorithm for estimating the ground state energy and for computing low energy states of quantum impurity models. Such models describe a bath of free fermions coupled to a small interacting subsystem called an impurity. The full system consists of $n$ fermionic modes and has a Hamiltonian $H = H_0 + H_{imp}$, where $H_0$ is quadratic in creation–annihilation operators and $H_{imp}$ is an arbitrary Hamiltonian acting on a subset of $O(1)$ modes. We show that the ground energy of $H$ can be approximated with an additive error $2^{-b}$ in time $n^3 \exp[O(b^3)]$. Our algorithm also finds a low energy state that achieves this approximation. The low energy state is represented as a superposition of $\exp[O(b^3)]$ fermionic Gaussian states.

To arrive at this result we prove several theorems concerning exact ground states of impurity models. In particular, we show that eigenvalues of the ground state covariance matrix decay exponentially with the exponent depending very mildly on the spectral gap of $H_0$. A key ingredient of our proof is Zolotarev’s rational approximation to the $\sqrt{x}$ function. We anticipate that our algorithms may be used in hybrid quantum-classical simulations of strongly correlated materials based on dynamical mean field theory. We implemented a simplified practical version of our algorithm and benchmarked it using the single impurity Anderson model.

Contents

1. Introduction ........................................ 452
   1.1 Main results .................................... 453
   1.2 Discussion and open problems ................. 456
   1.3 Miscellaneous results .......................... 457
2. Background ........................................ 458
   2.1 Canonical modes .............................. 458
   2.2 Pfaffians .................................... 459
   2.3 Gaussian unitary operators and gaussian states .... 460
1. Introduction

In this paper we study ground states and low energy states of quantum impurity models. Such models describe a bath of free fermions coupled to a small interacting subsystem called an impurity.

Hamiltonians of this form were famously studied in the 1960s and 70s by Anderson, Kondo, Wilson, and many others to investigate the physics of a magnetic impurity embedded in a metal [1–3]. This line of research elucidated the theoretical mechanism of the Kondo effect,\(^1\) which had been observed experimentally decades earlier [5]. It also spurred the development of Wilson’s numerical renormalization group [3], a non-perturbative numerical method that reproduces the low temperature physics of these systems.

The study of quantum impurity models extends beyond this direct application and provides a powerful numerical method for calculating electronic structure of strongly correlated materials such as transition metal compounds and high-temperature superconductors [6]. These materials are described by fermionic lattice models with interactions throughout the system, instead of localized within a small subsystem. Nevertheless, impurity models can be used to study such materials within an approximation known as dynamical mean field theory (DMFT) [7]. The impurity is typically chosen to model a group of atoms contained within a unit cell of the lattice, whereas the bath models the bulk of the material.

Recently there has been growing interest in solving impurity problems in the quantum information community. It was suggested by Bauer et al. [8] that a small quantum computer with a few hundred qubits can potentially speed up certain steps in material simulations based on the DMFT method. In particular, Ref. [8] proposed a quantum algorithm for computing the Green’s function of a quantum impurity model. Kreula et al. [9] subsequently proposed a proof-of-principle demonstration of this algorithm.

Quantum impurity problems are also interesting from the standpoint of Hamiltonian complexity theory [10]. In general, estimating the ground energy of a quantum

---

\(^1\) While it is generally expected that a metal should become a better conductor as temperature is reduced, for some metals with dilute impurities the resistivity achieves a minimum value at a nonzero temperature. In short, the resistivity can increase as temperature is lowered due to scattering of conduction electrons in the metal with a localized electron in the impurity (see, e.g., Ref. [4]).
many-body system composed of spins or fermi modes with local interactions is a hard problem. Formally, this problem is complete for the complexity class QMA—a quantum analogue of NP [11,12]. The QMA-completeness result implies that, in the worst case, the ground energy of interacting fermi systems cannot be computed efficiently (assuming QMA ≠ BQP). In contrast, Hamiltonians describing free fermions are exactly solvable and their ground energy can be computed in polynomial time. Quantum impurity models provide a natural arena for studying the complexity of fermionic systems in an intermediate regime interpolating between the free and the fully interacting cases.

In this paper we describe a classical algorithm for approximating the ground energy and for computing low energy states of quantum impurity models. We focus on the worst-case computational complexity of this problem as a function of the system size and the desired approximation error. We also prove several theorems concerning exact ground states of impurity models that appear to be new.

1.1. Main results. To state our results let us first define a general quantum impurity model. We consider the $2^n$-dimensional Hilbert space $\mathcal{H}_n$ of $n$ fermi modes, spanned by Fock basis vectors $|x_1, x_2, \ldots, x_n\rangle = (a_{x_1}^\dagger)(a_{x_2}^\dagger)\ldots(a_{x_n}^\dagger)|0^n\rangle$.

Here $a_j^\dagger$, $a_j$ are fermionic creation and annihilation operators, $x_j \in \{0, 1\}$ is the occupation number of the $j$th mode and $|0^n\rangle$ is the vacuum state which satisfies $a_j|0^n\rangle = 0$ for all $j$. A quantum impurity model is a Hamiltonian $H$ that acts on $\mathcal{H}_n$ as

$$H = H_0 + H_{imp},$$

where $H_0$ describes a bath of free fermions and $H_{imp}$ describes the impurity. To specify the form of $H_0$ and $H_{imp}$ it will be convenient to use Majorana operators $c_1, c_2, \ldots, c_{2n}$ defined by

$$c_{2j-1} = a_j + a_j^\dagger \quad \text{and} \quad c_{2j} = -i(a_j - a_j^\dagger). \quad (1)$$

The Majorana operators are hermitian and satisfy

$$c_p c_q + c_q c_p = 2\delta_{p,q} I \quad (2)$$

for all $1 \leq p, q \leq 2n$. We may write any free fermion Hamiltonian $H_0$ as

$$H_0 = e_0 I + \frac{i}{4} \sum_{p,q=1}^{2n} h_{p,q} c_p c_q, \quad (3)$$

where $h$ is real anti-symmetric matrix and $e_0 = \|h\|_1/4$ is an energy shift chosen such that $H_0$ has zero ground energy. Here and in the following we use $\| \cdot \|_1$ to denote the trace norm, while $\| \cdot \|$ denotes the operator norm. Let us choose the energy scale such that $\|h\| \leq 1$. Then single-particle excitation energies of $H_0$ belong to the interval $[0, 1]$ while eigenvalues of $H_0$ belong to the interval $[0, n]$.

Let us agree that $H_{imp}$ acts non-trivially only on the Majorana modes $c_1, \ldots, c_m$. Here $m$ is the impurity size. We shall be interested in the case $m \ll n$. The impurity Hamiltonian must include only even-weight Majorana operators (i.e., fermionic parity parity.
is conserved) but otherwise can be completely arbitrary. We may write the impurity Hamiltonian as

$$H_{imp} = \sum_{x \in \{0, 1\}^m} g_x e^{x_1} e^{x_2} \cdots e^{x_m},$$

where $g_x$ are some coefficients.\(^2\) We do not impose any restrictions on the magnitude of these coefficients or on the norm of $H_{imp}$. Let us write

$$e_g = \min_{\phi \in \mathcal{H}_n} \frac{\langle \phi | H | \phi \rangle}{\langle \phi | \phi \rangle}$$

for the ground energy of the full Hamiltonian. Our main result is as follows.

**Theorem 1** (Quasipolynomial algorithm). There exists a classical algorithm which takes as input a quantum impurity model $H$, a target precision $\gamma \in (0, 1/2]$, and outputs an estimate $E$ such that $|E - e_g| \leq \gamma$. The algorithm has runtime

$$O(n^3) \exp \left[ O(m \log^3 (m \gamma^{-1})) \right].$$

For a fixed impurity size $m$ the runtime is polynomial in $n$ and quasi-polynomial in $\gamma^{-1}$. We are not aware of any obstacles to achieving a polynomial scaling in $\gamma^{-1}$ and leave this as an open problem. On the other hand, the dependence of the runtime on $n$ and $m$ is nearly optimal. Indeed, choosing $H_0 = 0$ and $H_{imp} = 0$ reduces the problem to approximating the ground energy of $H_{imp}$ and $H_0$ respectively. In the worst case this requires time $2\Omega(m)$ and $\Omega(n^3)$ respectively (using existing methods). As far as we know, our algorithm is the first proposed method that gives a rigorous bound on the approximation error for general impurity models.

The proof of Theorem 1 including a complete description of the algorithm is given in Sect. 4.2. At a high level the algorithm proceeds as follows. We introduce a deformed impurity problem in which the single-particle energies of the bath Hamiltonian are approximated by a set of equally spaced grid points.\(^3\) This deformed impurity problem has a special feature that a large number of fermionic modes can be decoupled from the impurity by a (Gaussian) unitary transformation. We show that the full Hamiltonian $H$ has a low-energy state within a subspace $\mathcal{V}$ spanned by eigenstates of the deformed bath Hamiltonian such that (a) bath modes coupled to the impurity have at most $O(m \log^2 (m \gamma^{-1}))$ excitations and (b) all decoupled modes are unoccupied. We show that the dimension of $\mathcal{V}$ has no dependence on $n$. We approximate the ground energy $e_g$ by restricting the deformed impurity model onto the subspace $\mathcal{V}$ and using exact diagonalization to compute the smallest eigenvalue. The corresponding smallest eigenvector $\psi \in \mathcal{V}$ can be written as a superposition of at most $\dim(\mathcal{V})$ fermionic Gaussian states.

The analysis of our algorithm relies on new results concerning ground states of quantum impurity models; in particular, Theorem 2 (described below) and its corollaries. A simplified practical version of our algorithm is described in Sect. 5 and benchmarked using the single impurity Anderson model [1].

\(^2\) In order for $H_{imp}$ to be hermitian, the coefficients $g_x$ must be real for $|x| = 0 \pmod{4}$ and imaginary for $|x| = 2 \pmod{4}$.

\(^3\) We note that a discretization of the bath Hamiltonian is also used in the numerical renormalization group method [3].
Remark. The runtime quoted in Theorem 1 counts the total number of elementary algebraic operations $+,\times,/,$ $\sqrt{\cdot}$. Moreover, for the sake of readability, throughout the paper we ignore errors incurred in the standard linear algebra subroutines. In particular, we assume that eigenvalues of a hermitian $N \times N$ matrix $A$ can be computed exactly in time $O(N^3)$. Strictly speaking, the cost of this computation has a mild dependence on the desired precision and the norm of $A$. Applying Householder transformations to make $A$ tri-diagonal and using rigorous eigenvalue algorithms for tri-diagonal matrices [13] one can estimate all eigenvalues of $A$ with an additive error $\delta$ in time $O(N^3)\text{poly}(\log(N),\log(\delta^{-1}),\log(\|A\|))$, see Theorem 7.1 of Ref. [13]. Taking into account this overhead would alter the asymptotic runtime stated in Theorem 1 by a factor $\text{poly}(\log(n),\log(\|H_{imp}\|))$.

Let us now discuss ground states of quantum impurity models and their features. Since impurity models are usually not exactly solvable, their ground states lack an analytic expression. Moreover, even if an analytic expression could be found, it would likely depend on subtle details of the impurity Hamiltonian $H_{imp}$ which would limit its utility. A natural question is whether ground states posses some universal features that depend only on the bath Hamiltonian $H_0$ and the size of the impurity $m$. In this paper we provide one example of such a universal feature. To state our result consider an arbitrary impurity model $H = H_0 + H_{imp}$. Choose a new set of creation-annihilation operators $b_j^\dagger, b_j$ that diagonalize the bath Hamiltonian:

$$H_0 = \sum_{j=1}^{n} \epsilon_j b_j^\dagger b_j, \quad 0 \leq \epsilon_j \leq 1.$$  

Here $\epsilon_j$ are single-particle excitation energies of the bath. The fact that $\epsilon_j \in [0,1]$ follows from our assumption that $\|h\| \leq 1$, see the remarks after Eq. (3). Let $\omega > 0$ be the spectral gap of the bath. That is, each $\epsilon_j$ is either zero or contained in the interval $[\omega,1]$.

**Theorem 2 (Exponential Decay).** There exists a ground state $\psi$ of $H$ such that the following holds. Let $C$ be a hermitian $n \times n$ matrix defined by

$$C_{ik} = \langle \psi | b_i^\dagger b_k | \psi \rangle \quad (4)$$

and let $\sigma_1 \geq \sigma_2 \geq \cdots \sigma_n \geq 0$ be its eigenvalues. Then for all $j$

$$\sigma_j \leq c \exp \left[ - \frac{j}{14m \log(2\omega^{-1})} \right]. \quad (5)$$

Here $c > 0$ is some universal constant.

Assuming that the impurity has a constant size $m = O(1)$, the theorem asserts that the eigenvalues of the ground state covariance matrix decay exponentially with an exponent that depends very mildly on the spectral gap of the bath. Moreover, if all excitation energies of the bath are strictly positive, we show that Eqs. (4, 5) hold for any ground state $\psi$ of $H$. Let us emphasize that the exponential decay Eq. (5) is a universal feature.

---

4 In certain cases one can compute the ground energy of quantum impurity models exactly in the thermodynamic limit $n \to \infty$ using the Bethe Ansatz method [14,15]. This method is applicable only if the couplings between the bath and the impurity have a certain special symmetry and the bath has a linear dispersion law.
of a ground state that has no dependence on $H_{imp}$. Also we note that Theorem 2 assumes nothing about the spectrum of the full Hamiltonian $H$.

An important corollary of Theorem 2 is that an exact ground state of $H$ can be well approximated by a superposition of a small number of fermionic Gaussian states. Indeed, we show that all excitations present in the bath can be “localized” on a small subset of modes by some Gaussian unitary operator. Informally, each zero eigenvalue of the covariance matrix $C$ can be identified with an empty fermionic mode $|0\rangle$ (after a suitable Gaussian unitary transformation). Thus, if $C$ has at most $k$ non-zero eigenvalues, at least $n-k$ modes must be in the vacuum state. Any state of the remaining $k$ modes can be written as a superposition of at most $2^k$ Gaussian states. Choosing a suitable cutoff value to truncate small eigenvalues of $C$ yields a good approximation of $\psi$ by a superposition of a few Gaussian states, see Sect. 3 for details. Theorem 2 plays a central role in the analysis of our quasi-polynomial algorithm.

The proof of Theorem 2 proceeds in two steps. First we use a variational characterization of ground states to show that the covariance matrix $C$ must be a feasible solution of a certain semidefinite program that depends only on $H_0$ and the linear subspace spanned by the impurity modes. Secondly, we prove that any feasible solution $C$ of this program exhibits an exponential decay of eigenvalues as stated in Eq. (5). This step exploits the machinery of rational approximations developed by Zolotarev [16] in 1877—an extension of Chebyshev’s well-known theory of polynomial approximation. A formal proof of the theorem is presented in Sect. 3.1.

1.2. Discussion and open problems. We have shown that the structure of quantum impurity models can be exploited to enable fast computation of the ground energy and low energy states. Our work may find application in the hybrid quantum-classical DMFT algorithm proposed by Bauer et al. in Ref. [8]. This algorithm has two steps which are performed on a quantum computer. The first step is to prepare a ground state $\psi$ of a quantum impurity model. Bauer et al. suggest using quantum adiabatic evolution followed by phase estimation for the state preparation [8]. The second step is to compute the impurity model Green’s functions; in this step one simulates Schrödinger time evolution with the quantum impurity model Hamiltonian starting from a state simply related to $\psi$. Our work suggests that the state preparation step can be simplified by classically computing an approximate version of the ground state $\psi$. This approximate ground state is specified as a superposition of a small number of Gaussian states and can be prepared efficiently on a quantum computer using techniques discussed in “Appendix B”. This would obviate the need for the quantum adiabatic evolution—a heuristic which usually cannot be rigorously justified due to a lack of lower bounds on the minimal spectral gap.

One may ask: is there a good classical algorithm to simulate the time evolution of quantum impurity models? If so, this might obviate the need for the second step of the algorithm from Ref. [8]. As we now explain, a recent work by Brod and Childs [17] provides evidence that such efficient classical simulation may not be possible. Consider a system of $n$ qubits and Hamiltonian

$$H(t) = g(t)(X_{n-2}X_n + Y_{n-2}Y_n) + \sum_{i=1}^{n-2} f_i(t)(X_iX_{i+1} + Y_iY_{i+1}).$$

(6)

Here $f_i(t), g(t)$ are time-dependent coefficients and $X_j, Y_j$ are the Pauli operators acting on the $j$th qubit. Section IV of Ref. [17] shows that Schrödinger time evolution with the
above Hamiltonian can efficiently simulate a quantum computation on $\Omega(n)$ qubits. The Hamiltonian Eq. (6) can be rewritten in terms of Majorana operators \{c_1, c_2, \ldots, c_{2n}\} using the standard Jordan–Wigner transformation (see Eqs. (149–152)); it takes the form of a quantum impurity model with impurity size $m = 6$:

$$H(t) = -g(t)(c_{2n-4}c_{2n-1}c_{2n-3}c_{2n-2} - c_{2n-5}c_{2n-3}c_{2n-2} - 2) - i \sum_{j=1}^{n} f_j(t)c_{2j}c_{2j+1}.$$ 

Putting this together we see that Schrödinger time evolution with a \textit{time-dependent} impurity model Hamiltonian can perform efficient universal quantum computation (and is therefore unlikely to be efficiently classically simulable). It is an open question whether or not a time-independent impurity Hamiltonian can also perform efficient universal quantum computation.

The most direct open question raised by our work is whether or not our bounds can be improved. For example, we do not know if the exponential decay stated in Theorem 2 can be strengthened, for example, by eliminating the dependence on the spectral gap of the bath $\omega$. A related question is whether or not there is an algorithm for estimating the ground energy of quantum impurity problems which scales polynomially as a function of $\gamma^{-1}$ (where $\gamma$ is the desired precision).

Our results demonstrate that a ground state of a quantum impurity model can be approximated by a superposition of a small number of fermionic Gaussian states. In Sect. 5, we describe a simplified practical version of our algorithm which is based on using such states as a variational ansatz. The algorithm allows one to minimize the energy of an arbitrary fermionic Hamiltonian with quadratic and quartic interactions over superpositions of $\chi$ Gaussian states, where $\chi$ is a fixed parameter. We hope that this variational algorithm may be useful in other contexts beyond the study of quantum impurity models. For example, in quantum chemistry, the Hartree-Fock approximation is based on minimizing the energy of a fermionic Hamiltonian over Slater determinant states. A generalized Hartree-Fock method proposed by Kraus and Cirac in Ref. [18] is a variational algorithm that minimizes the energy within the larger class of Gaussian states. In contrast to Slater determinants, Gaussian states are capable of describing certain correlations between electrons such as emergence of Cooper pairs in the BCS theory of superconductivity. Our work extends the algorithm of Ref. [18] to arbitrary superpositions of $\chi$ Gaussian states. In Sect. 5, we use the single impurity Anderson model [1] as a toy model to benchmark our variational algorithm. We found that the $\chi = 2$ algorithm approximates the ground energy within the first eight significant digits for $n \leq 40$.

1.3. Miscellaneous results. In this section we collect results that are not directly related to our quasi-polynomial algorithm. These results provide additional insights on the structure of ground states of quantum impurity models and the complexity of estimating their ground energy.

\textbf{Efficient algorithm for gapped impurity models:} The algorithm from Theorem 1 does not require any condition on the spectral gap of the quantum impurity model Hamiltonian. We show that if the full Hamiltonian $H$ has a constant spectral gap then its ground energy can be approximated efficiently using a different technique.

\textbf{Theorem 3.} Suppose the impurity has size $m = O(1)$. Suppose the full Hamiltonian $H$ has a non-degenerate ground state and a constant energy gap above the ground state.
Then there exists a classical algorithm that approximates the ground energy \( e_g \) within a given precision \( \delta \) in time \( \text{poly}(n, \delta^{-1}) \).

The proof of the theorem is given in Sect. 4.3. It proceeds by establishing an efficiently computable mapping (unitary transformation) between the impurity model and a Hamiltonian which describes a chain of \( O(n) \) qudits with nearest neighbor interactions and maximum qudit dimension \( 2^m \). The mapping does not require any condition on the gap, and since it is unitary the spectrum of the two models coincide. In the gapped case the ground energy can be computed efficiently using known algorithms for 1D gapped systems [19].

**Approximation with inverse polynomial precision:** Let us now consider the complexity of estimating the ground energy of a quantum impurity model to inverse polynomial precision. Formally, consider a decision version of the problem:

**Quantum impurity problem.** We are given a quantum impurity model \( H \) with \( n \) fermi modes and impurity size \( m = O(1) \), and two energy thresholds \( a < b \) such that \( b - a = 1/\text{poly}(n) \). We are promised that either \( e_g \leq a \) (yes instance) or \( e_g \geq b \) (no instance) and asked to decide which is the case.

Note that the algorithm from Theorem 1 has quasipolynomial run time if \( \gamma \) scales inverse polynomially with \( n \). Although our algorithm is not efficient in this precision regime, we are able to prove the following complexity upper bound.

**Theorem 4.** The quantum impurity problem is contained in QCMA.

The proof of Theorem 4 is given in “Appendix B”. Here QCMA is a quantum analog of NP [20]. Roughly speaking, it consists of those decision problems where every yes instance has a polynomial-sized classical proof which can be efficiently verified using a quantum computer.

### 2. Background

To make the paper self-contained, in this section we briefly summarize some basic facts concerning free fermion Hamiltonians and fermionic Gaussian states. The material of this section is mostly based on Refs. [21,22].

**2.1. Canonical modes.** Consider a quadratic Hamiltonian

\[
H_0 = e_0 I + \frac{i}{4} \sum_{p,q=1}^{2n} h_{p,q} c_p c_q
\]

where \( h \) is a real anti-symmetric matrix and \( e_0 \) is an energy shift chosen such that \( H_0 \) has zero ground energy. Given a complex vector \( x \in \mathbb{C}^{2n} \), define an operator

\[
b(x) = \sum_{j=1}^{2n} x_j c_j.
\]

Let us say that \( b(x) \) is a **canonical mode** of \( H_0 \) if

\[
[H_0, b(x)] = -\epsilon b(x), \quad \epsilon \geq 0.
\]
Majorana commutation rules Eq. (2) give

\[ [H_0, b(x)] = i b(hx), \]

that is, \( x \) must be an eigenvector of \( h \) with an eigenvalue \( i \epsilon \). Furthermore, since \( b(x) \) reduces the energy of any eigenvector of \( H_0 \) by \( \epsilon \) and \( b(x)^2 \) is proportional to the identity due to Eq. (2), we conclude that \( b(x)^2 = 0 \) whenever \( \epsilon > 0 \). Choosing an orthonormal set of eigenvectors of \( h \) and noting that

\[ \{b^\dagger(x), b(y)\} = \{b(x^*), b(y)\} = 2 \sum_{j=1}^{2n} x^*_j y_j \]

one can construct a complete set of canonical modes \( b_1, \ldots, b_n \) such that

\[ H_0 = \sum_{j=1}^{n} \epsilon_j b^\dagger_j b_j, \quad \epsilon_j \geq 0, \quad (8) \]

\[ b_j^2 = 0, \quad \{b_i, b_j\} = \delta_{i,j} I. \quad (9) \]

Specifically, if \( u_1, \ldots, u_n \in \mathbb{C}^{2n} \) are orthonormal eigenvectors of \( h \) such that \( hu_j = i \epsilon_j u_j \) with \( \epsilon_j \geq 0 \) then \( b_j = b(u_j) \). We shall refer to the operators \( b_1, \ldots, b_n \) constructed above as canonical modes of \( H_0 \). Canonical modes can be computed in time \( O(n^3) \) by diagonalizing \( h \).

2.2. Pfaffians. Suppose \( n = 2k \) and \( M \in \mathbb{C}^{n \times n} \) is a complex anti-symmetric matrix. The Pfaffian of \( M \) denoted \( \text{Pf} (M) \) is a complex number defined as

\[ \text{Pf} (M) = \frac{1}{2^k k!} \sum_{\sigma \in S_n} (-1)^\sigma M_{\sigma(1), \sigma(2)} \cdots M_{\sigma(n-1), \sigma(n)}. \quad (10) \]

Here the sum runs over the symmetric group \( S_n \) and \( (-1)^\sigma \) is the parity of a permutation \( \sigma \). Let us agree that \( \text{Pf} (M) = 0 \) whenever \( M \) has odd size. For small \( n \) one can compute Pfaffians directly from the definition:

\[ n = 2 : \text{Pf} (M) = M_{1,2} \]
\[ n = 4 : \text{Pf} (M) = M_{1,2} M_{3,4} - M_{1,3} M_{2,4} + M_{1,4} M_{2,3} \quad (11) \]

The well-known properties of the Pfaffian are

\[ \text{Pf} (M)^2 = \det (M) \quad (12) \]

and

\[ \text{Pf} \left( RMR^T \right) = \det (R) \text{Pf} (M) \quad (13) \]

for any complex matrix \( R \). Using Eq. (12) one can compute \( \text{Pf} (M) \) up to an overall sign in time \( O(n^7) \). Most of the algorithms for computing the Pfaffian proceed by transforming
$M$ into a tri-diagonal form \cite{23,24}. This transformation gives a complex matrix $R$ whose determinant is easy to compute such that

\[ RM R^T = \sum_{p=1}^{n-1} x_p (|p\rangle \langle p+1| - |p+1\rangle \langle p|) \]  

(14)

for some complex coefficients $x_p$. Definition Eqs. (10) and (13) then imply that

\[ \text{Pf} (M) = \det (R) \cdot (x_1 x_3 \cdots x_{n-1}). \]  

(15)

From Eqs. (14, 15) one can compute $\text{Pf} (M)$ including the overall sign using $O(n^3)$ arithmetic operations. A detailed discussion of algorithms and optimized implementations can be found in Ref. \cite{23}.

2.3. Gaussian unitary operators and gaussian states. A unitary operator $U$ acting on the Fock space $\mathcal{H}_n$ is called Gaussian if its conjugated action maps any Majorana operator $c_p$ to a linear combination of Majorana operators $c_1, \ldots, c_{2n}$ that is,

\[ U c_p U^\dagger = \sum_{q=1}^{2n} R_{p,q} c_q \]  

(16)

for some real orthogonal matrix $R$. Gaussian unitary operators form a group $C_n$ which coincides with $O(2n)$ if one ignores the overall phase of operators. The group $C_n$ is generated by operators $U = \exp \left( \frac{i}{2} c_p c_q \right)$ that implement rotations

\[ U c_p U^\dagger = \cos (\theta) c_p - \sin (\theta) c_q \quad \text{and} \quad U c_q U^\dagger = \sin (\theta) c_p + \cos (\theta) c_q. \]

and by reflection-like operators $U = c_p$ that flip the sign of all $c_q$ with $q \neq p$.

A state $\phi \in \mathcal{H}_n$ is called Gaussian if it is obtained from the vacuum state $|0^n\rangle$ by a Gaussian unitary, i.e., $|\phi\rangle = U |0^n\rangle$ for some $U \in C_n$. Let $\mathcal{G}_n$ be the set of all Gaussian states. Any state $\phi \in \mathcal{G}_n$ can be specified up to an overall phase by its covariance matrix $M$ of size $2n \times 2n$ which is defined as

\[ M_{p,q} = (-i/2) \langle \phi | (c_p c_q - c_q c_p) |\phi\rangle. \]  

(17)

By definition, $M$ is a real anti-symmetric matrix. For example, a Fock basis state $|y\rangle$ has a block-diagonal covariance matrix

\[ M_y \equiv \bigoplus_{j=1}^{n} \begin{bmatrix} 0 & (-1)^{y_j+1} \langle -1|^{y_j} \\ (-1)^{y_j+1} \langle -1|^{y_j} & 0 \end{bmatrix}. \]  

(18)

A Gaussian state $|\phi\rangle = U |y\rangle$ has covariance matrix $M = R M_y R^T$, where $R \in O(2n)$ is defined by Eq. (16). This implies that a valid covariance matrix must satisfy $M^2 = -I$. Conversely, any real anti-symmetric matrix $M$ such that $M^2 = -I$ is a covariance matrix of some Gaussian state.

\footnote{Gaussian unitary operators are sometimes called canonical or Bogolyubov transformations.}
Let $N = \sum_{j=1}^{n} a_j^\dagger a_j$ be the particle number operator and

$$P = (-1)^N = (-i)^n c_1 c_2 \cdots c_{2n-1} c_{2n}$$

be the fermionic parity operator. Note that any Gaussian unitary $U \in \mathcal{C}_n$ either commutes or anti-commutes with $P$ since the generators $\exp(\theta \sum c_p c_q)$ and $c_p$ commute and anti-commute with $P$ respectively. Since $P |0^n\rangle = |0^n\rangle$, it follows that any Gaussian state $\phi \in \mathcal{G}_n$ has a fixed parity: $P \phi = \sigma \phi$ for some $\sigma = \pm 1$. From Eq. (13) one infers that $\sigma = Pf(M)$, where $M$ is the covariance matrix of $\phi$. We shall say that $\phi$ is even (odd) if $\sigma = 1 (\sigma = -1)$. Gaussian states that are eigenvectors of the number operator $N$ are sometimes called Slater determinants.

We shall say that a state $\psi \in \mathcal{H}_n$ has a Gaussian rank $\chi$ if it can be written as a superposition of at most $\chi$ Gaussian states. Gaussian rank is analogous to the Slater number studied in Ref. [25]. We shall be mostly interested in low-rank Gaussian states, that is, states with Gaussian rank $\chi = O(1)$ independent of $n$.

Expectation value of any observable on a Gaussian state $\phi \in \mathcal{G}_n$ can be efficiently computed using Wick’s theorem. By linearity, it suffices to consider observables proportional to Majorana monomials

$$c(x) = c_1^{x_1} c_2^{x_2} \cdots c_{2n}^{x_{2n}}, \quad x_p \in \{0, 1\}.$$ 

(20)

Such monomials form an orthogonal basis in the algebra of operators acting on $\mathcal{H}_n$. Wick’s theorem can be stated in terms of Pfaffians defined in Sect. 2.2 as

$$\langle \phi | c(x) | \phi \rangle = Pf (i M[x]) \quad \text{for all } x,$$

(21)

where $\phi$ is a Gaussian state, $M$ is the covariance matrix of $\phi$, and $M[x]$ is a submatrix of $M$ that includes only rows and columns $j$ such that $x_j = 1$. For example,

$$\langle \phi | c_p c_q c_r c_s | \phi \rangle = -(M_{p,q} M_{r,s} - M_{p,r} M_{q,s} + M_{p,s} M_{q,r})$$

for any $p < q < r < s$. Note also that $\langle \phi | P | \phi \rangle = Pf (M)$.

Let $H_0$ be a quadratic Hamiltonian considered in Sect. 2.1 and $b_1, \ldots, b_n$ be its canonical modes. Let us order the canonical modes such that

$$0 \leq \epsilon_1 \leq \epsilon_2 \leq \cdots \leq \epsilon_n$$

and let $k$ be the number of zero-energy modes, that is, $\epsilon_1 = \cdots = \epsilon_k = 0$ and $\epsilon_{k+1} > 0$. Then the ground subspace of $H_0$ has a form

$$\ker (H_0) = \text{span}(U|x_1, \ldots, x_k, 0, 0, \ldots, 0) : x_i \in \{0, 1\}),$$

where $U \in \mathcal{C}_n$ is a Gaussian unitary such that $b_j = U a_j U^\dagger$ for all $j$. In particular, if $H_0$ has no zero-energy modes then its unique ground state is $U |0^n\rangle$. The parity of $U |0^n\rangle$ is determined by the sign of $Pf (h)$, see [26] for more details.
2.4. Inner product formulas. In this section we state several useful formulas for various inner products that involve Gaussian states. They can be viewed as a slightly generalized version of the standard inner product formulas for Slater determinants \cite{27}. For the sake of completeness we provide a proof of all formulas in “Appendix A”.

Consider Gaussian states \( \phi_1, \phi_2 \in \mathcal{G}_n \) with the same parity \( \sigma \) and let \( \rho_a = |\phi_a\rangle \langle \phi_a| \). Let \( M_a \) be the covariance matrix of \( \rho_a \). The magnitude of the inner product \( \langle \phi_1 | \phi_2 \rangle \) is given by

\[
|\langle \phi_1 | \phi_2 \rangle|^2 = \text{Tr}(\rho_1 \rho_2) = \sigma 2^{-n} \cdot \text{Pf}(M_1 + M_2). \tag{22}
\]

Furthermore, \( \text{Tr}(\rho_1 \rho_2) = 0 \) if \( \phi_0, \phi_1 \) have different parity.

Suppose \( \text{Tr}(\rho_1 \rho_2) \neq 0 \). Can we compute the inner product \( \langle \phi_1 | \phi_2 \rangle \) including the overall phase? To make this question meaningful, first we need to specify a Gaussian state including the overall phase. To this end, let us fix some reference state \( \phi_0 \in \mathcal{G}_n \), for example the vacuum state or a randomly chosen Gaussian state. We shall specify a Gaussian state \( \phi \in \mathcal{G}_n \) by its covariance matrix \( M \) and by its inner product with the reference state \( \langle \phi_0 | \phi \rangle \). Here we assume that \( \phi \) and \( \phi_0 \) are not orthogonal. We show that

\[
\langle \phi_0 | \phi_1 \rangle \cdot \langle \phi_1 | \phi_2 \rangle \cdot \langle \phi_2 | \phi_0 \rangle = \sigma 4^{-n} i^n \text{Pf} \left( \begin{array}{ccc} iM_0 & -I & I \\ I & iM_1 & -I \\ -I & I & iM_2 \end{array} \right) 
\]

where \( \phi_a \in \mathcal{G}_n \) are Gaussian states with covariance matrices \( M_a \) and parity \( \sigma \). If states \( \phi_0, \phi_1, \phi_2 \) do not have the same parity then at least one inner product \( \langle \phi_a | \phi_b \rangle = 0 \) and the righthand side of Eq. (23) is zero. One can rewrite Eq. (23) in a more compact form that only involves Pfaffians of matrices of size \( 2n \),

\[
\langle \phi_0 | \phi_1 \rangle \cdot \langle \phi_1 | \phi_2 \rangle \cdot \langle \phi_2 | \phi_0 \rangle = 4^{-n} \cdot \text{Pf}(M_1 + M_2) \cdot \text{Pf}(\Delta + M_0) \tag{24}
\]

where

\[
\Delta = (-2I + iM_1 - iM_2)(M_1 + M_2)^{-1}. \tag{25}
\]

Note that \( M_1 + M_2 \) is invertible if \( \phi_1, \phi_2 \) are not orthogonal, see Eq. (22). One can easily check that \( \Delta \) is an anti-symmetric matrix (use the identity \( M_a^2 = -I \)). Using Eqs. (23, 24) one can compute the inner product \( \langle \phi_1 | \phi_2 \rangle \) including the overall phase in time \( O(n^3) \).

In order to compute matrix elements \( \langle \phi_1 | c(x) | \phi_2 \rangle \) we shall need a generalized Wick’s theorem that involves a pair of Gaussian states. Suppose \( x \in \{0, 1\}^{2n} \) is an even-weight string and let \( w = |x| \) be its Hamming weight. Define a matrix \( J_x \) of size \( w \times 2n \) such that \( (J_x)_{i,j} = 1 \) if \( j \) is the position of the \( i \)-th nonzero element of \( x \) and \( (J_x)_{i,j} = 0 \) otherwise. Define a diagonal matrix \( D_x \) if size \( 2n \times 2n \) such that \( (D_x)_{i,j} = 1 - x_j \). For example, if \( x = 0^{2n} \) then \( D_x = I \) and \( J_x \) is an empty matrix. We will show that

\[
\langle \phi_0 | \phi_1 \rangle \cdot \langle \phi_1 | c(x) | \phi_2 \rangle \cdot \langle \phi_2 | \phi_0 \rangle = \sigma 4^{-n} i^n \text{Pf} (R_x), \tag{26}
\]

where

\[
R_x = \begin{bmatrix}
         iM_0 & -I & I \\
         I & iM_1 & -I \\
         -I & I & iM_2 \\
       \end{bmatrix}
\]

\[
J_x^I \quad iD_xM_2J_x^I
\]

\[
-J_x + iJ_xM_2D_x \\
iJ_xM_2J_x^I
\]

is an anti-symmetric matrix of size \( 6n + w \). As before, \( \sigma = \pm 1 \) is the common parity of \( \phi_0, \phi_1, \phi_2 \).
In the special case when $\phi_1, \phi_2$ are not orthogonal one can use a simplified formula

\[
\frac{\text{Tr}(\rho_2 \rho_1 c(x))}{\text{Tr}(\rho_2 \rho_1)} = \text{Pf} \left( i \Delta[x]^* \right).
\]  

Here $\Delta$ is defined by Eq. (25) and $\Delta[x]$ is a submatrix of $\Delta$ that includes only rows and columns from the support of $x$. We use a notation $\Delta^*$ for the complex conjugate matrix. Furthermore, if $M_1 = M_2 = M$ then $\Delta = M$ so that Eq. (27) reduces to the standard Wick’s theorem, see Eq. (21). Note that Eq. (27) can be rewritten as

\[
\langle \phi_1 | c(x) | \phi_2 \rangle = \langle \phi_1 | \phi_2 \rangle \cdot \text{Pf} \left( i \Delta[x]^* \right).
\]

Computing the inner product $\langle \phi_1 | \phi_2 \rangle$ using Eq. (23) or Eq. (24) this gives $\langle \phi_1 | c(x) | \phi_2 \rangle$. Note that once the matrix $\Delta$ has been computed, Eq. (24) determines the inner product $\langle \phi_1 | \phi_2 \rangle$, and thus Eq. (27) enables computation of $\langle \phi_1 | c(x) | \phi_2 \rangle$ in time $O(|x|^3)$ independent of $n$ for any $x$. This is particularly useful when $c(x)$ describes a single term in some fermionic Hamiltonian $H$. In this case $x$ usually has Hamming weight $O(1)$ and one can compute $\langle \phi_1 | H | \phi_2 \rangle$ in time $O(k)$, where $k$ is the number of terms in $H$. To the best of our knowledge, Eqs. (23, 24, 26, 27) are new.

3. Ground States of Quantum Impurity Models

In this section we study exact ground states of quantum impurity models and establish some of their features. We prove Theorem 2 and discuss its implications for the approximation of ground states by superpositions of Gaussians. We will also see how bath excitations can be “localized” by a Gaussian unitary operator.

3.1. Proof of Theorem 2. Let $b_j$ and $\epsilon_j$ be the canonical modes and single-particle excitation energies of the bath Hamiltonian $H_0$, see Sect. 2.1. Then

\[
H_0 = \sum_{j=1}^{n} \epsilon_j b_j^\dagger b_j, \quad 0 \leq \epsilon_j \leq 1.
\]

We shall first assume that $\epsilon_j \geq \omega > 0$ for all $j = 1, 2, \ldots, n$. In this case we will show that Eq. (5) holds for any ground state $\psi$ of $H$. At the end of the proof we handle the case where one or more single particle excitation energy is zero and we show that in this case Eq. (5) holds for at least one ground state of $H$.

For any complex vector $x \in \mathbb{C}^n$ define a fermionic operator

\[
b(x) \equiv \sum_{j=1}^{n} x_j b_j.
\]

Recall that the impurity is formed by the first $m$ Majorana modes $c_1, \ldots, c_m$. Define a linear subspace $\mathcal{L} \subseteq \mathbb{C}^n$ such that $x \in \mathcal{L}$ iff the expansion of $b(x)$ in terms of the Majorana operators $c_1, \ldots, c_{2n}$ does not include $c_1, \ldots, c_m$. We note that

\[
\dim (\mathcal{L}) \geq n - m
\]  

since $\mathcal{L}$ is described by $m$ linear constraints on $n$ variables $x_1, \ldots, x_n$. Majorana commutation rules $c_p c_q = -c_p c_q$ for $p \neq q$ imply that $b(x)$ anti-commutes with $c_1, \ldots, c_m$.
whenever \( x \in L \). Since \( H_{\text{imp}} \) includes only even-weight monomials in \( c_1, \ldots, c_m \), we get
\[
[H_{\text{imp}}, b(x)] = 0 \quad \text{for all } x \in L. \tag{29}
\]

Suppose \( \psi \) is any normalized ground state of \( H \). Then
\[
\langle \psi | b(x) \dagger [b(x), H] | \psi \rangle \leq 0. \tag{30}
\]

since \( b(x) \psi \) cannot have energy smaller than \( \psi \). Combining this and Eq. (29) we conclude that
\[
\langle \psi | b(x) \dagger [b(x), H_0] | \psi \rangle \leq 0 \quad \text{for all } x \in L. \tag{31}
\]

Using the commutation rules \([b_j, b_k \dagger b_k] = \delta_{j,k} b_j \) one gets
\[
\sum_{j,k=1}^n \bar{x}_j x_k \epsilon_k \langle \psi | b_j \dagger b_k | \psi \rangle \leq 0 \quad \text{for all } x \in L. \tag{32}
\]

Define a ground state covariance matrix \( C \) and a single-particle energy matrix \( E \) such that
\[
C_{j,k} = \langle \psi | b_j \dagger b_k | \psi \rangle \quad \text{and} \quad E_{j,k} = \epsilon_j \delta_{j,k}. \tag{33}
\]

Since for now we assume all single particle energies are at least \( \omega \) we have
\[
\omega I \leq E \leq I. \tag{34}
\]

We note that
\[
0 \leq C \leq I \tag{35}
\]

Indeed, \( C \geq 0 \) since \( C \) is a covariance matrix. Commutation rules \( b_j \dagger b_k + b_k b_j \dagger = \delta_{j,k} I \) and the assumption \( \langle \psi | \psi \rangle = 1 \) imply that \( (I - C)_{j,k} = \langle \psi | b_k b_j \dagger | \psi \rangle \), that is, \( I - C \geq 0 \) which proves Eq. (35). Next we observe that \( CE \) must have a real non-positive expectation value on any vector \( x \in L \) due to Eq. (32). Equivalently, a restriction of \( CE \) onto \( L \) defines a hermitian negative semi-definite matrix. Denoting \( \Lambda \) a projector onto \( L \) one can rewrite Eq. (32) in a matrix form as
\[
\Lambda (CE - EC) \Lambda = 0 \quad \text{and} \quad \Lambda CE \Lambda \leq 0. \tag{36}
\]

Finally,
\[
\text{rank}(\Lambda) \geq n - m \quad \text{and} \quad \Lambda^2 = \Lambda. \tag{37}
\]

due to Eq. (28). We shall use Eqs. (34–37) to prove the following lemma. It establishes a bound slightly stronger than Eq. (5) in the case where \( \epsilon_j \geq \omega \) for all \( j \).

**Lemma 1.** Let \( \Lambda, C, E \) be \( n \times n \) hermitian matrices and \( \omega \) be a positive number such that Eqs. (34, 35, 36, 37) are satisfied. Let \( \sigma_1 \geq \sigma_2 \geq \ldots \geq \sigma_n \) be the eigenvalues of \( C \). Then for all \( j \)
\[
\sigma_j \leq c \exp \left[ -\frac{j}{7m \log (2\omega^{-1})} \right]. \tag{38}
\]

Here \( c > 0 \) is some universal constant.
Proof. Let us first sketch the main steps of the proof. Suppose one can find a subspace $\mathcal{D} \subseteq \mathcal{L}$ such that
\[ [C, E^{1/2}] \cdot \mathcal{D} = 0. \tag{39} \]
Here and below we define the square root $E^{1/2}$ such that its eigenvalues are non-negative. Let $\Delta$ be the projector onto $\mathcal{D}$. Clearly, $\Delta E^{1/2}C E^{1/2} \Delta \geq 0$ since $C \geq 0$. On the other hand,
\[ \Delta E^{1/2}C E^{1/2} \Delta = \Delta C E \Delta - \Delta[C, E^{1/2}] E^{1/2} \Delta = \Delta C E \Delta \]
due to Eq. (39). The inclusion $\mathcal{D} \subseteq \mathcal{L}$ and Eq. (36) imply $\Delta C E \Delta = \Delta \Delta C E \Delta \leq 0$ and thus
\[ \Delta E^{1/2}C E^{1/2} \Delta \leq 0. \tag{40} \]
To avoid a contradiction one has to assume that $\Delta E^{1/2}C E^{1/2} \Delta = 0$. Since $C \geq 0$, this is possible only if $E^{1/2} \cdot \mathcal{D} \subseteq \ker(C)$. If the subspace $\mathcal{D}$ is sufficiently large, this would show that $C$ has sufficiently many zero eigenvalues. Unfortunately, we do not know how to construct a subspace satisfying Eq. (39) exactly. Instead we shall realize an approximate version of Eq. (39). In other words, we shall construct a subspace $\mathcal{D} \subseteq \mathcal{L}$ and a hermitian operator $Z$ acting on $\mathbb{C}^n$ such that
\[ [C, Z] \cdot \mathcal{D} = 0 \quad \text{and} \quad Z \approx E^{1/2}. \tag{41} \]
The desired operator $Z$ will be constructed using a low-degree rational approximation to the square root function due to Zolotarev [16]. This approximation has a form
\[ x^{1/2} \approx \frac{x P_d(x)}{Q_d(x)} \quad \text{for } \omega \leq x \leq 1 \]
where $P_d(x), Q_d(x)$ are degree-$d$ polynomials and the approximation error scales as $\exp \left[ -cd / \log (2\omega^{-1}) \right]$ for some constant $c > 0$. (For comparison, approximating $x^{1/2}$ by the Taylor series at $x = 1$ truncated at some order $d$ achieves an approximation error $\exp \left[ -cd\omega \right]$ which is significantly worse if $\omega$ is small.) We shall approximate $E^{1/2}$ by an operator $Z = EP_d(E)Q_d^{-1}(E)$. Let us write
\[ Z = M_1 M_2 \cdots M_{2d+1}, \tag{42} \]
where each $M_i$ is a “monomial” $M_i = E + \lambda_i I$ or $M_i = (E + \lambda_i I)^{-1}$ for some real numbers $\lambda_i$. A subspace $\mathcal{D} \subseteq \mathcal{L}$ satisfying Eq. (41) is constructed in two steps. First, construct a subspace $\mathcal{D}_0 \subseteq \mathcal{L}$ such that $[C, E] \cdot \mathcal{D}_0 = 0$. We shall choose $\mathcal{D}_0$ as the intersection of $\mathcal{L}$ and $\ker((C, E))$. Second, define
\[ \mathcal{D} = \mathcal{D}_0 \cap \left( M_1^{-1} \mathcal{D}_0 \right) \cap \left( M_2^{-1} M_1^{-1} \mathcal{D}_0 \right) \cap \cdots \cap \left( M_{2d+1}^{-1} \cdots M_2^{-1} M_1^{-1} \mathcal{D}_0 \right). \tag{43} \]
We claim that $[C, Z] \phi = 0$ for any state $\phi \in \mathcal{D}$. Using the chain rule for the commutator $[C, Z] = [C, M_1 \cdots M_{2d+1}]$ it suffices to check that
\[ [C, M_{j+1}] M_j \cdots M_2 M_1 \phi = 0 \quad \text{for all } \phi \in \mathcal{D} \]
for all $j$. Suppose first that $M_{j+1} = E + \lambda_{j+1} I$. By construction of $\mathcal{D}$, there exists a state $\phi' \in \mathcal{D}_0$ such that $\phi = M_j^{-1} \cdots M_2^{-1} M_1^{-1} \phi'$. Since all $M$’s commute, one has
\[ [C, M_{j+1}] M_j \cdots M_2 M_1 \phi = [C, M_{j+1}] \phi' = [C, E] \phi' = 0 \]
since $\phi' \in \mathcal{D}_0$ and $[C, E] \cdot \mathcal{D}_0 = 0$. Suppose next that $M_{j+1} = (E + \lambda_{j+1} I)^{-1}$. Then

$$[C, M_{j+1}] M_j \cdots M_2 M_1 \phi = -M_{j+1} [C, M_{j+1}^{-1}] M_j \cdots M_2 M_1 \phi.$$  

Again, by construction of $\mathcal{D}$, there exists $\phi' \in \mathcal{D}_0$ such that $\phi = M_{j+1}^{-1} \cdots M_2^{-1} M_1^{-1} \phi'$. Taking into account that $M_{j+1}^{-1} = E + \lambda_{j+1} I$ one gets

$$[C, M_{j+1}] M_j \cdots M_2 M_1 \phi = -M_{j+1} [C, M_{j+1}^{-1}] \phi' = -M_{j+1} [C, E] \phi' = 0$$  

since $\phi' \in \mathcal{D}_0$ and $[C, E] \cdot \mathcal{D}_0 = 0$. This proves that $[C, Z] \cdot \mathcal{D} = 0$ as promised. How large is the subspace $\mathcal{D}$? We shall use the fact that $\mathcal{L}$ has dimension at least $n - m$ to show that $\mathcal{D}_0$ has dimension at least $n - 3m$ and $\mathcal{D}$ has dimension $r \geq n - 6md + O(1)$. Repeating the steps that lead to Eq. (40) with $E^{1/2}$ replaced by $Z$ we will show that $\Delta E^{1/2} CE^{1/2} \Delta$ has an exponentially small norm. We then use Cauchy’s interlacing theorem to show that $C$ has at least $r = n - O(md)$ eigenvalues with magnitude at most $\exp \left[ -cd / \log (2\omega^{-1}) \right]$. Since we are free to choose $d$ arbitrarily, this is possible only if the eigenvalues of $C$ decay exponentially.

Let us now proceed to a formal proof of Lemma 1. Define a subspace

$$\mathcal{D}_0 = \mathcal{L} \cap \ker (CE - EC)$$  

and let $\Delta_0$ be the projector on $\mathcal{D}_0$. By definition, $[C, E] \Delta_0 = 0$. From Eqs. (36, 37) one infers that the commutator $[C, E]$ has rank at most $2m$, that is, $\ker (CE - EC)$ has dimension at least $n - 2m$. Therefore

$$\dim (\mathcal{D}_0) \geq \dim (\mathcal{L}) + \dim (\ker [C, E]) - n \geq (n - m) + (n - 2m) - n = n - 3m.$$  

We conclude that any matrix $C$ that satisfies Eqs. (35, 36) must also satisfy

$$0 \leq C \leq I$$  

$$CE - EC \Delta_0 = 0$$  

$$\Delta_0 CE \Delta_0 \leq 0$$  

and

$$\operatorname{rank}(\Delta_0) \geq n - 3m.$$  

Here in the third line we noted that $\Delta_0 CE \Delta_0$ is a restriction of a negative semi-definite operator $\Delta CE \Delta$ onto $\mathcal{D}_0$. Our goal is to show that any matrix $C$ satisfying Eqs. (45–47) has exponentially decaying eigenvalues as claimed in Eq. (38).

We shall approximate the matrix square root $E^{1/2}$ by rational functions of a sufficiently small degree. Optimal rational approximations of a given degree to the sign and square root functions were found in 1877 by Zolotarev [16]. They have been used in more recent times for high-energy physics simulations, see [28, 29]. The following lemma quantifies the quality of Zolotarev’s approximation.

**Lemma 2 (Zolotarev’s approximation).** For any integer $d \geq 1$ and real number $0 < \omega < 1$ there exist degree-$d$ polynomials $P_d(x), Q_d(x)$ such that

$$\left| \sqrt{x} - x \frac{P_d(x)}{Q_d(x)} \right| \leq 2\sqrt{x} \cdot \exp \left[ -\frac{d}{\log (2\omega^{-1})} \right].$$  

for all $x \in [\omega, 1]$. All roots of the polynomials $P_d(x)$ and $Q_d(x)$ are negative real numbers.
It should be pointed out that the construction of the polynomials $P_d(x), Q_d(x)$ depends on $\omega$. For the sake of readability we omit the dependence of $P_d(x), Q_d(x)$ on $\omega$ in our notations. Since the proof of Lemma 2 is a simple combination of known facts [30,31], we postpone it until Sect. 3.2. This section also provides explicit formulas for the roots of $P_d(x), Q_d(x)$. We note that it is possible to improve the exponent on the right-hand side of Eq. (49) to $-d\pi^2/\log(256\omega^{-1})$ (see the proof), but for ease of notation we use the above bound.

We shall use Zolotarev’s approximations to prove the following.

**Proposition 1.** Let $d \geq 1$ be any integer and let $r \equiv n - 6m(d + 1)$. Then there exists a projector $\Delta$ of rank at least $r$ such that any solution $C$ of Eqs. (45–47) obeys

$$\|\Delta C\| \leq 10\exp\left[-\frac{d}{\log(2\omega^{-1})}\right].$$

(50)

**Proof.** Consider some fixed integer $d$ and a gap $\omega > 0$ such that all eigenvalues of $E$ lie in the interval $[\omega, 1]$. Let $P_d, Q_d$ be the degree-$d$ polynomials from Lemma 2 such that $xP_d(x)Q_d^{-1}(x)$ approximates $x^{1/2}$ for all $\omega \leq x \leq 1$. Define

$$Z \equiv EP_d(E)Q_d^{-1}(E).$$

Then Lemma 2 implies

$$Z = E^{1/2}(I + A), \quad \|A\| \leq 2\exp\left[-\frac{d}{\log(2\omega^{-1})}\right].$$

(51)

Without loss of generality we shall assume that the right hand side of Eq. (51) is at most $\frac{1}{2}$, forcing $\|A\| \leq \frac{1}{2}$. Indeed, if the right hand side of Eq. (51) is larger than $\frac{1}{2}$, the right-hand side of Eq. (50) is $> 1$ and the proposition holds trivially. Defining $B = (I + A)^{-1} - 1$ and rearranging Eq. (51) we get

$$E^{1/2} = Z(I + B), \quad \|B\| = \|A(I + A)^{-1}\| \leq 2\|A\|.$$  

(52)

Moreover, the operators $Z, A, B, E$ are diagonal over the same basis and mutually commute.

We may decompose

$$Z = \prod_{i=1}^{2d+1} M_i$$

(53)

where $M_i = E + \lambda_i I$ or $M_i = (E + \lambda_i I)^{-1}$. The operators $M_i$ are hermitian and nonsingular since all roots of $P_d, Q_d$ lie on the negative real axis while $E \geq \omega I > 0$. Furthermore, all monomials $M_i$ commute with each other. Let $D \subseteq D_0$ be the subspace defined by Eq. (43). We claim that

$$\dim(D) \geq n - 6m(d + 1).$$

(54)

Indeed, since $D_0$ has dimension at least $n - 3m$, the orthogonal complement $D_0^\perp$ has dimension at most $3m$. Likewise, the orthogonal complement to $(M_j^{-1} \cdots M_i^{-1}D_0)^\perp$ has dimension at most $3m$. Since $D^\perp$ is contained in the sum of $2d + 2$ subspaces $D_0^\perp$ and $(M_j^{-1} \cdots M_i^{-1}D_0)^\perp$ with $j = 1, \ldots, 2d + 1$, see Eq. (43), one infers that $D^\perp$ has
dimension at most $3m(2d + 2)$. This proves Eq. (54). Below we assume that $d$ is small enough such that $\mathcal{D}$ is non-empty. Let $\Delta$ be the projector onto $\mathcal{D}$.

The arguments below Eq. (43) prove that $C$ commutes with $Z$ if restricted onto the subspace $\mathcal{D}$, that is,
\begin{equation}
[C, Z]_{\Delta} = 0.
\end{equation}

Using Eqs. (51, 55) and the fact that $E, A, Z$ mutually commute we obtain
\begin{align}
\Delta E^{1/2}C E^{1/2} &= \Delta E^{1/2} CZ \Delta - \Delta E^{1/2} C E^{1/2} A \Delta \\
&= \Delta E^{1/2} Z C \Delta - \Delta E^{1/2} C AE^{1/2} \Delta \\
&= \Delta E^{1/2} E^{1/2} (I + A) C \Delta - \Delta E^{1/2} C AE^{1/2} \Delta \\
&= \Delta E C \Delta + \Delta E^{1/2} A E^{1/2} C \Delta - \Delta E^{1/2} C AE^{1/2} \Delta 
\end{align}
\begin{equation}
(56)
\end{equation}

Here the first line uses $E^{1/2} = Z - E^{1/2} A$. Again using the fact that $E, A, Z, B$ mutually commute along with Eqs. (51, 52, 55) to rearrange the second term:
\begin{align}
\Delta E^{1/2} A E^{1/2} C \Delta &= \Delta E^{1/2} A(I + B) Z C \Delta \\
&= \Delta E^{1/2} A(I + B) C Z \Delta \\
&= \Delta E^{1/2} A(I + B) C(I + A) E^{1/2} \Delta 
\end{align}
\begin{equation}
(57)
\end{equation}

Combining Eqs. (56, 57) gives
\begin{equation}
\Delta E^{1/2} C E^{1/2} - \Delta E C \Delta = \Delta E^{1/2} \left( A(I + B) C(I + A) - CA \right) E^{1/2} \Delta 
\end{equation}
\begin{equation}
(58)
\end{equation}

From Eqs. (46, 47) and $\Delta \leq \Delta_{0}$ we infer that $\Delta E C \Delta$ is Hermitian and negative semidefinite. Using this fact in Eq. (58) we obtain the operator inequality
\begin{align}
\Delta E^{1/2} C E^{1/2} \Delta &\leq \Delta E^{1/2} \left( A(I + B) C(I + A) - CA \right) E^{1/2} \Delta \\
&\leq \|A(I + B) C(I + A) - CA\| \\
&\leq \|A(I + B) C(I + A)\| + \|CA\|.
\end{align}
\begin{equation}
(59)
\end{equation}

Let $\Delta'$ be the projector onto the support of $E^{1/2} \Delta E^{1/2}$. From Eq. (59) one gets
\begin{align}
\|\Delta' C \Delta'\| &= \max_{\phi \in \Delta} \frac{\langle \phi | E^{1/2} C E^{1/2} | \phi \rangle}{\langle \phi | E | \phi \rangle} \\
&\leq \max_{\phi \in \Delta} \frac{\langle \phi | E^{1/2} (A(I + B) C(I + A) - CA) E^{1/2} | \phi \rangle}{\langle \phi | E | \phi \rangle} \\
&\leq \|A(I + B) C(I + A) - CA\| \\
&\leq \|A(I + B) C(I + A)\| + \|CA\|.
\end{align}
\begin{equation}
(60)
\end{equation}

Noting that $\|I + B\|, \|I + A\| \leq 2$ and $\|C\| \leq 1$, and using Eq. (51) to bound $\|A\|$ we get
\begin{equation}
\|\Delta' C \Delta'\| \leq 10 \exp \left[ - \frac{d}{\log (2\omega^{-1})} \right].
\end{equation}
\begin{equation}
(61)
\end{equation}

Since $E$ is invertible, $\Delta'$ has rank at least $n - 6m(d + 1)$, see Eq. (54). This proves Eq. (50) with $\Delta = \Delta'$. \hfill \Box
We can now complete the proof of Lemma 1. Note that it suffices to consider the case where 

\[ j \geq c_1 m \]

for some universal constant \( c_1 \). Indeed, we may then choose the constant \( c \) in Eq. (38) to satisfy \( c > e^{c_1/7 \log(2)} \); with this choice for all \( j \leq c_1 m \) the right hand side of Eq. (38) is \( \geq 1 \) and the claim holds trivially.

Let \( \Delta \) be the projector of rank \( r \geq n - 6m(d + 1) \) from Proposition 1. Let \( \sigma_j(C) \) and \( \sigma_j(\Delta C \Delta) \) be the \( j \)-th largest eigenvalues of the respective operators. Cauchy’s interlacing theorem implies

\[ \sigma_j(C) \leq \sigma_{j-(n-r)}(\Delta C \Delta). \]

Choose

\[ d + 1 = \left\lfloor \frac{j - 1}{6m} \right\rfloor \]

so that \( r \geq n - j + 1 \). Note that we may choose a universal constant \( c_1 \) such that \( d \geq j/7m \) for all \( j \geq c_1 m \). Then, for all \( j \geq c_1 m \), Proposition 1 gives

\[ \sigma_j(C) \leq \sigma_{j-(n-r)}(\Delta C \Delta) \leq \sigma_1(\Delta C \Delta) = \| \Delta C \Delta \| \leq 10 \exp \left( -\frac{j}{7m \log (2\omega - 1)} \right). \]

As noted above, it is sufficient to establish the bound only for \( j \geq c_1 m \). This proves the lemma. \( \Box \)

Let us now handle the case when \( H_0 \) has zero-energy modes. Suppose

\[ \epsilon_1 = \epsilon_2 = \cdots = \epsilon_T = 0 \]

and \( \epsilon_j \geq \omega \) for \( j > T \). We shall first reduce to the case where the total number \( T \) of zero energy modes satisfies \( T \leq m \).

Recall the subspace \( \mathcal{L} \subseteq \mathbb{C}^n \) defined around Eq. (29). Define another linear subspace \( Q \subseteq \mathbb{C}^n \) such that \( x \in Q \) iff \( x_j = 0 \) for all \( j > T \). We have

\[ \dim(\mathcal{L} \cap Q) \geq T - m \]

since \( \dim(\mathcal{L}) \geq n - m \) and \( \dim(Q) = T \). Note that \( [b(x), H_0] = 0 \) for all \( x \in Q \) and \( [b(x), H_{imp}] = 0 \) for all \( x \in \mathcal{L} \) and therefore

\[ [b(x), H] = 0 \quad \text{for all } x \in \mathcal{L} \cap Q. \]

We may form a \( T \times T \) unitary matrix \( U \) where the rows (when padded with \( n - T \) zeros) span \( Q \) and the first \( \dim(\mathcal{L} \cap Q) \) rows span \( \mathcal{L} \cap Q \). The new modes

\[ \tilde{b}_j = \begin{cases} \sum_{k=1}^T U_{jk} b_k & j = 1, \ldots, T \\ b_j & T < j \leq n \end{cases} \]

then satisfy

\[ [\tilde{b}_j, H] = 0 \quad \text{for all } j = 1, \ldots, T - m. \]
Thus we may write \( H = I \otimes H' \) where \( H' = H'_0 + H'_\text{imp} \) describes the nontrivial action of \( H \) on modes \( \tilde{b}_j \) for \( j > T - m \). Here \( H'_0 \) has \( m \) zero energy modes and spectral gap \( \omega \). We may therefore choose a ground state \( \psi \) of the full Hamiltonian \( H \) which satisfies \( |\psi \rangle = |\tilde{0}^{(T-m)} \otimes \phi \rangle \) where \( \phi \) is a ground state of \( H' \) and \( \tilde{0}^{(T-m)} \) is the vacuum state for all modes \( \tilde{b}_j \) with \( j \leq (T - m) \).

The covariance matrix \( \tilde{C} \) of \( \psi \) defined with respect to the new modes, i.e.,

\[
\tilde{C}_{jk} = \langle \psi | \tilde{b}_j \tilde{b}_k | \psi \rangle
\]

is unitarily equivalent to the matrix \( C \) defined in Eq. (4) and therefore has the same spectrum. Moreover, \( \tilde{b}_j | \psi \rangle = 0 \) for all \( j \leq (T - m) \) and therefore

\[
\tilde{C} = \begin{pmatrix}
0_{(T-m) \times (T-m)} & 0_{(T-m) \times (n+m-T)} \\
0_{(n+m-T) \times (n+m-T)} & C'
\end{pmatrix}
\]

where \( C' \) is the covariance matrix for \( \phi \). Thus, to prove Theorem 2 for the original impurity model \( H \) it suffices to prove that Eq. (5) holds for \( C' \), the covariance matrix of an (arbitrary) ground state \( \phi \) of \( H' \). This shows that without loss of generality we may consider the case where \( T \leq m \).

To complete the proof it remains to handle the case where \( E \) has at most \( m \) zero eigenvalues and all other eigenvalues are at least \( \omega \). In this case we show that Eq. (5) holds for all ground states \( \psi \) of \( H \). Define a subspace

\[
L' = L \cap \ker (E)^\perp.
\]

Recall that \( \dim (L) \geq n - m \). Then \( L' \) has dimension at least \( n - 2m \). Let \( \Lambda' \) be the projector onto \( L' \), so

\[
\text{rank}(\Lambda') \geq n - 2m.
\]

Define a deformed energy matrix \( E' \) by setting \( \epsilon_j = \omega \) for \( j = 1, \ldots, m \). Now

\[
\omega I \leq E' \leq I.
\]

Furthermore, \( E \Lambda' = E' \Lambda' \). Combining this and Eq. (35) gives

\[
\Lambda'(C'E' - E'C)\Lambda' = 0 \quad \text{and} \quad \Lambda'C E' \Lambda' \leq 0.
\]

Now apply Lemma 1 with \( \Lambda \) and \( E \) replaced by \( \Lambda' \) and \( E' \), and with \( m \) replaced by \( 2m \). This gives Eq. (5) and completes the proof.

Remark: We observe that Eqs. (35, 36) define a semi-definite program (SDP) with a variable \( C \). The SDP depends on the energy matrix \( E \) and the projector \( \Lambda \). Thus the ground state covariance matrix \( C \) must be a feasible solution of the SDP. Choosing an objective function to be maximized one can extract some useful information about ground states of a particular impurity model. For example, maximizing \( \text{Tr}(C) \) subject to Eqs. (35, 36) provides an upper bound on the average number of excitations in the bath since \( \text{Tr}(C) = \langle \psi | \sum_{j=1}^n b_j^\dagger b_j | \psi \rangle \). We observed numerically that this upper bound is typically much better than what one would expect from our general results, e.g. Lemma 1. In fact, for the vast majority of impurity models that we examined (but not for all) we observed that \( \text{Tr}(C) \leq 2m \) regardless of the gap of \( H_0 \).
3.2. Rational approximations to the square root function. In this section we prove Lemma 2 and provide explicit formula for the roots of the polynomials $P_d(x), Q_d(x)$. For convenience, we repeat the statement of the lemma.

**Lemma 2** (Zolotarev’s approximation). For any integer $d \geq 1$ and real number $0 < \omega < 1$ there exist degree-$d$ polynomials $P_d(x), Q_d(x)$ such that

$$\left| \sqrt{x} - x \frac{P_d(x)}{Q_d(x)} \right| \leq 2 \sqrt{x} \cdot \exp \left[ -\frac{d}{\log (2\omega^{-1})} \right].$$

(49) for all $x \in [\omega, 1]$. All roots of the polynomials $P_d(x)$ and $Q_d(x)$ are negative real numbers.

**Proof.** We shall need bounds on the convergence of Zolotarev’s approximations to the sign function. The following fact was proved in Ref. [30] and stated more explicitly in Ref. [31] (see page 9).

**Fact 1.** For each $0 < \delta < 1$ and integer $d \geq 1$ there exist degree-$d$ polynomials $P_d, Q_d$ such that

$$\max_{x \in J(\delta)} \left| \frac{\operatorname{sgn}(x) - x P_d(x^2)}{Q_d(x^2)} \right| \leq 2 \exp \left[ -\frac{d\pi K(\sqrt{1 - \mu^2})}{4K(\mu)} \right].$$

(62)

Here $J(\delta) = [-1, -\delta] \cup [\delta, 1], \mu = \frac{1 - \sqrt{\delta}}{1 + \sqrt{\delta}}$ (63) and $K(\mu)$ is the complete elliptic integral of the first kind:

$$K(\mu) = \int_0^{\pi/2} \frac{d\theta}{\sqrt{1 - \mu^2 \sin^2(\theta)}}$$

Furthermore, all roots of $P_d$ and $Q_d$ are real and non-positive.

The lemma follows easily from the above fact. Indeed, let $r(d, \delta)$ be right-hand side of Eq. (62). Then

$$\left| |x| - x^2 \frac{P_d(x^2)}{Q_d(x^2)} \right| = |x| \cdot \left| \frac{\operatorname{sgn}(x) - xP_d(x^2)}{Q_d(x^2)} \right| \leq |x| \cdot r(d, \delta)$$

for all $x \in J(\delta)$. Changing variables $y = x^2$ one gets

$$\left| \sqrt{y} - y \frac{P_d(y)}{Q_d(y)} \right| \leq \sqrt{y} \cdot r(d, \sqrt{\omega})$$

(64)

for all $\omega \leq y \leq 1$. It remains to explicitly compute the error bound $r(d, \delta)$. We shall use some bounds on the elliptic integrals from Ref. [32]. Define

$$F(\mu) = \frac{\pi}{2} \frac{K(\sqrt{1 - \mu^2})}{K(\mu)}.$$ 

Using equations (1.3, 1.5) from [32] we have

$$F(\mu) = \frac{\pi^2}{2F\left(\frac{1-\mu}{1+\mu}\right)} = \frac{\pi^2}{2F(\sqrt{\delta})}.$$ 

(65)
Now equation (1.6) from [32] states that $F(r) < \log(4/r)$ for all $r \in (0, 1)$. Using this bound in the denominator of Eq. (65) gives

$$F(\mu) > \frac{\pi^2}{\log(16\delta^{-1})}.$$ We arrived at

$$r(d, \delta) = 2 \exp \left[ -\frac{d}{2} F(\mu) \right] \leq 2 \cdot \exp \left[ -\frac{d\pi^2}{2 \log(16\delta^{-1})} \right],$$

and therefore

$$r(d, \sqrt{\omega}) \leq 2 \cdot \exp \left[ -\frac{d\pi^2}{\log(16\delta^{-1})} \right] \leq 2 \cdot \exp \left[ -\frac{d\pi^2}{8 \log(2\omega^{-1})} \right].$$

Substituting this into Eq. (64) and using the fact that $\pi^2/8 > 1$ completes the proof. □

Next let us describe an explicit construction of the polynomials $P_d(x)$, $Q_d(x)$ from Lemma 2. This material is based on Refs. [16,30,31]. Below we assume that $0 < \omega \leq 1$. Define

$$\mu \equiv \sqrt{1 - \omega}.$$ We shall need Jacobi elliptic functions $\text{sn}(u; \mu)$ and $\text{cn}(u; \mu)$. They are defined for $u \geq 0$ by

$$\text{sn}(u; \mu) = \sin (\phi(u)) \quad \text{and} \quad \text{cn}(u; \mu) = \cos (\phi(u)),$$

where $\phi(u) \geq 0$ is the unique solution of

$$u = \int_0^{\phi(u)} \frac{d\theta}{\sqrt{1 - \mu^2 \sin^2(\theta)}}.$$

For each $j = 1, \ldots, 2d$ define

$$\lambda_j = \omega \left[ \frac{\text{sn}\left(\frac{jK(\mu)}{2d+1}; \mu\right)}{\text{cn}\left(\frac{jK(\mu)}{2d+1}; \mu\right)} \right]^2. \quad (66)$$

Define

$$M = 2 \left[ \prod_{j=1}^{2d} \frac{1 + \lambda_{2j}}{1 + \lambda_{2j-1}} + \sqrt{\omega} \prod_{j=1}^{2d} \frac{\omega + \lambda_{2j}}{\omega + \lambda_{2j-1}} \right]^{-1}.$$

Then

$$P_d(x) = M \prod_{j=1}^{d} (x + \lambda_{2j}) \quad \text{and} \quad Q_d(x) = \prod_{j=1}^{d} (x + \lambda_{2j-1}). \quad (67)$$

The coefficients $\lambda_j$ can be easily computed using any computer algebra system such as MATLAB. We plot the worst-case relative error

$$r(\omega, d) \equiv \max_{\omega \leq x \leq 1} x^{-1/2} \left| x^{1/2} - xP_d(x)Q_d^{-1}(x) \right|$$

(68)
as a function of $\omega$ for a few small values of $d$ on Fig. 1.

Finally, let us point out that $\sqrt{x}$ can be approximated by a rational function of a given degree $d$ on the full interval $[0, 1]$. However, in this case the approximation error decays exponentially with $\sqrt{d}$. A simple example of such approximation has been proposed by Newman [33] (although Ref. [33] concerns with approximating the $|x|$ function, a simple change of variable shows that the same results hold for $\sqrt{x}$). In contrast, Zolotarev’s approximation holds only on the interval $\omega \leq x \leq 1$ but the approximation error decays exponentially with $d$. Ref. [33] also demonstrates that rational approximations can be exponentially more accurate compared with the polynomial approximations of the same degree.

3.3. Approximation by low-rank Gaussian states. In this section we derive two corollaries of Theorem 2 that characterize ground states of quantum impurity models. Let $\psi$ be some ground state of the full Hamiltonian $H$ and $C$ be the covariance matrix of $\psi$ defined in Theorem 2. It is not hard to see that, roughly speaking, eigenvalues of $C$ are related to the number of bath excitations present in $\psi$. For example, $\text{Tr}(C)$ is the expected value of the number operator $\sum_j b_j^\dagger b_j$ in the state $\psi$. In the extreme case when $\text{Tr}(C) = 0$ the ground state $\psi$ itself is a Gaussian state (the ground state of $H_0$). More generally, the exponential decay stated in Theorem 2 is sufficient to show that $\psi$ is approximated by a relatively small number $\chi \ll 2^n$ of Gaussian states. Furthermore, all excitations present in the bath can be “localized” on a small subset of modes by some Gaussian unitary operator. Recall that $\omega$ denotes the spectral gap of $H_0$.

**Corollary 1.** There exists a ground state $\psi$ of $H$ such that the following holds. For any $\delta > 0$ there exists an integer

$$
k = 28m \log (2\omega^{-1}) \left[ \log (\delta^{-1}) + \log (m) + \log \log (2\omega^{-1}) + O(1) \right], \quad (69)$$

a Gaussian unitary operator $U$, and some (non-Gaussian) state $\phi \in \mathcal{H}_k$ such that

$$
\|\psi - U|\phi \otimes 0^{n-k}\| \leq \delta. \quad (70)
$$
Proof. Let $\psi$ and $C$ be the state and corresponding matrix from Theorem 2. Let $V$ be a unitary operator such that

$$V^\dagger CV = \sum_{j=1}^n \sigma_j |j\rangle\langle j|, \quad \sigma_1 \geq \sigma_2 \geq \ldots \geq \sigma_n.$$  

Define a new set of fermi modes $\tilde{b}_1, \ldots, \tilde{b}_n$ such that $\tilde{b}_j = \sum_{k=1}^n V_{k,j} b_k$. Then

$$\langle \psi | \tilde{b}_j^\dagger \tilde{b}_j | \psi \rangle = \sigma_j \delta_{i,j}. \quad (71)$$

Define a projector $\Pi_j = \tilde{b}_j \tilde{b}_j^\dagger$ so that $\langle \psi | (I - \Pi_j) | \psi \rangle = \sqrt{\sigma_j}$ and thus

$$\|\psi - \Pi_n \Pi_{n-1} \cdots \Pi_{k+1} \psi\| \leq \sum_{j=k+1}^n \sqrt{\sigma_j} \leq O(1) \cdot m \log(2\omega^{-1})$$

and

$$\times \exp\left[-\frac{k}{28m \log(2\omega^{-1})}\right]$$

where in the last inequality we used Theorem 2. Thus

$$\|\psi - \Pi_n \Pi_{n-1} \cdots \Pi_{k+1} \psi\| \leq \delta/2$$

for $k$ given by Eq. (69). Choose

$$|\psi'\rangle = \gamma \Pi_n \Pi_{n-1} \cdots \Pi_{k+1} |\psi\rangle,$$

where $\gamma$ is the normalizing coefficient. The above shows that $\gamma^{-1} \geq 1 - \delta/2$. Thus $\psi'$ approximates $\psi$ within error $\delta$. Finally, since $\Pi_j$ projects onto a subspace in which the mode $\tilde{b}_j$ is empty, the state $\psi'$ is the vacuum state for the subset of $n - k$ fermi modes $\tilde{b}_n, \ldots, \tilde{b}_{k+1}$. Therefore $|\psi'\rangle = U |\phi \otimes 0^{n-k}\rangle$ for some Gaussian unitary operator $U$ and some (non-Gaussian) state $\phi \in \mathcal{H}_k$. $\square$

From Eq. (70) one infers that $\psi$ is $\delta$-close to a superposition of $\chi = 2^k$ Gaussian states where $k$ is defined by Eq. (69). The next corollary states our best asymptotic upper bound on the number of Gaussian states one needs to approximate an exact ground state within a specified precision. This corollary provides a partial justification for the variational algorithm of Sect. 5 that minimizes the energy of $H$ over low-rank superpositions of Gaussian states. It also confirms our intuition (stated above) that eigenvalues of $C$ are related to the number of bath excitations in the ground state.

**Corollary 2.** There exists a ground state $\psi$ of $H$ such that the following holds. For any $\delta \in (0, 1/2]$ there exists a normalized state $\phi \in \mathcal{H}_n$ such that $\|\phi - \psi\| \leq \delta$ and

$$|\phi\rangle = \sum_{a=1}^\chi z_a |\theta_a\rangle, \quad \chi = e^{O(m \log(\omega^{-1}) \log(k^{-1}))} \quad (72)$$

where $\theta_1, \ldots, \theta_\chi \in \mathcal{G}_n$ are orthonormal Gaussian states. Each state $\theta_a$ is an eigenvector of the particle number operator $N = \sum_{j=1}^n b_j^\dagger b_j$ such that

$$N|\theta_a\rangle = k_a |\theta_a\rangle, \quad k_a \leq cm \log(2\omega^{-1}) \log(\delta^{-1}). \quad (73)$$
Here \( c > 0 \) is a universal constant. Furthermore, the projector

\[
P \equiv \sum_{a=1}^{\chi} |\theta_a\rangle \langle \theta_a| \tag{74}
\]

commutes with \( H_{\text{imp}} \).

**Proof.** We shall reuse some definitions and notation from the proof of Theorem 2 (repeated here for convenience). For any complex vector \( x \in \mathbb{C}^n \) define a fermionic operator

\[
b(x) \equiv \sum_{j=1}^{n} x_j b_j.
\]

Each canonical bath mode \( b_j \) can be written as a linear combination of Majorana modes \( c_1, \ldots, c_{2n} \). Recall that the impurity is formed by the first \( m \) modes \( c_1, \ldots, c_m \). Define a linear subspace \( \mathcal{L} \subseteq \mathbb{C}^n \) such that \( x \in \mathcal{L} \) iff the expansion of \( b(x) \) in terms of the Majorana operators does not include \( c_1, \ldots, c_m \).

As noted in Eqs. (29, 28) we have \( [H_{\text{imp}}, b(x)] = 0 \) for all \( x \in \mathcal{L} \) and \( \dim(\mathcal{L}) \geq n - m \). Define \( \Lambda \) to be the projector onto \( \mathcal{L} \). Let \( C \) and \( \psi \) be as in Theorem 2. Write

\[
\lambda_1 \geq \lambda_2 \geq \cdots \lambda_n \geq 0
\]

for the eigenvalues of \( \Lambda C \Lambda \). By Cauchy’s interlacing theorem and Theorem 2 we have

\[
\lambda_i \leq \sigma_i \leq c \exp \left[ -\frac{i}{14m \log (2\omega^{-1})} \right],
\]

where \( \sigma_i \) is the \( i \)-th largest eigenvalue of \( C \). Let \( \{x^j : j \in [n]\} \) be an orthonormal basis of eigenvectors of \( \Lambda C \Lambda \), with

\[
\text{span}\{x^1, \ldots, x^L\} = \mathcal{L} \quad L = \dim \mathcal{L}.
\]

and \( \Lambda C \Lambda x^j = \lambda_j x^j \). Define a new set of creation-annihilation operators \( \hat{b}^+_j, \hat{b}_j \) such that

\[
\hat{b}_j = b(x^j) = \sum_{k=1}^{n} x^j_k b_k \quad j = 1, 2, \ldots, n.
\]

We have

\[
[\hat{b}_j, H_{\text{imp}}] = 0 \quad j = 1, 2, \ldots, L. \tag{75}
\]

Now divide up the set of positive integers into intervals of size \( \sim 14m \log(2\omega^{-1}) \). That is, let \( Q = \lceil 14m \log(2\omega^{-1}) \rceil \) and define

\[
I_1 = \{1, 2, \ldots, Q\}
\]
\[
I_2 = \{Q + 1, \ldots, 2Q\}
\]
\[
I_3 = \{2Q + 1, \ldots, 3Q\}
\]
\[
:\]

Let \([L] \equiv \{1, 2, \ldots, L\}\). For each positive integer \(s\) define

\[ N_s = \sum_{j \in I_s \cap [L]} \hat{b}_j^+ \hat{b}_j. \]

There are \(\sim L/Q\) of these operators which are nonzero. Also note that Eq. (75) implies

\[ [N_s, H_{imp}] = 0 \quad (76) \]

for all \(s\). We have

\[ \langle \psi | N_k | \psi \rangle = \sum_{j \in I_k \cap [L]} \lambda_j \leq c_0 m \log(2\omega^{-1}) e^{-(k-1)} \quad (77) \]

where \(c_0\) is another universal constant. Since the operators \(\{N_k\}\) mutually commute, we can view \(\psi\) as inducing a probability distribution \(\Psi\) given by

\[ \Psi(n_1, n_2 \ldots) = \langle \psi | M_{n_1, n_2, \ldots} | \psi \rangle \]

where \(M_{n_1, n_2, \ldots}\) is the projector onto Fock basis states with simultaneous eigenvalues \(n_1, n_2, \ldots\) for operators \(N_1, N_2, \ldots\). Define

\[ R_k = c_0 m \log(2\omega^{-1}) e^{-(k-1)/2} \quad \text{and} \quad p_k = \frac{R_k}{Q} \leq c_1 e^{-(k-1)/2} \]

where \(c_1\) is another universal constant. From Markov’s inequality and Eq. (77) we obtain

\[ \Pr[\Psi(n_k \geq R_k)] \leq e^{-(k-1)/2}. \]

Applying a union bound we arrive at

\[ \Pr[\Psi(n_k \leq R_k \text{ for all } k \geq J)] \geq 1 - \sum_{j \geq J} e^{-(j-1)/2} \]

Let us choose \(J\) so that

\[ \sum_{j \geq J} e^{-(j-1)/2} \leq \delta^2/2 \quad \text{and} \quad p_k < \frac{1}{2} \quad \text{for all } k \geq J, \quad (78) \]

i.e., \(J = O(\log(\delta^{-1}))\). Then

\[ \Pr[\Psi(n_k \leq R_k \text{ for all } k \geq J)] \geq 1 - \delta^2/2. \]

Given a binary string \(\theta \in \{0, 1\}^n\) let \(|\theta\rangle \in \mathcal{H}_n\) be the Fock basis vector with respect to the modes \(\hat{b}_1, \ldots, \hat{b}_n\). In other words, \(\hat{b}_j^+ \hat{b}_j |\theta\rangle = \theta_j |\theta\rangle\) for all \(j\). Define a projector \(P\) onto a linear subspace

\[ \text{span} \left( |\theta\rangle : N_k |\theta\rangle = n_k |\theta\rangle, \quad n_k \leq R_k \quad \text{for } J \leq k \leq n \right). \quad (79) \]

From the above we have \(\langle \psi | P | \psi \rangle \geq 1 - \delta^2/2\). Defining \(|\phi\rangle = \|P | \psi\rangle\|^{-1} P | \psi\rangle\) we therefore have

\[ \|\psi - \phi\|^2 \leq 2(1 - \sqrt{1 - \delta^2/2}) \leq \delta^2. \]
Thus $\psi$ is $\delta$-close to $\phi$. We now show that $P$ projects onto a space of dimension upper bounded as

$$e^{O(m \log(\omega^{-1}) \log(\delta^{-1}))}.$$  

Fock basis states $|\theta\rangle$ in the image of $P$ are indexed by bit strings of length $n$ where the last $n - L$ bits are unrestricted while the first $L$ bits are divided up into the intervals $I_s \cap [L]$. The hamming weight of $\theta$ in interval $I_s$ is required to be at most $R_s$ when $s \geq J$. Letting $F(m, l)$ denote the number of bit strings of length $m$ with hamming weight at most $l$ we obtain

$$\text{Tr}(P) \leq 2^{(n-L)2Q(J-1)} \prod_{k \geq J} F(Q, R_k) \leq 2^{m+Q(J-1)} \prod_{k \geq J} F(Q, R_k),$$

where in the second inequality we used the fact that $L \geq n - m$. Recall that $p_k = R_k/Q$. Since $p_k < 1/2$ for all $k \geq J$ we may bound

$$F(Q, R_k) = \sum_{s=0}^{R_k} \binom{Q}{s} \leq 2^{H(p_k)Q} \text{ for all } k \geq J$$

where $H(p) = -p \log_2(p) - (1 - p) \log_2(1 - p)$ is the binary entropy function. Therefore

$$\text{Tr}(P) \leq 2^{m+Q(J-1)+Q \sum_{k \geq J} H(p_k)} \quad (80)$$

Now using the inequality $H(x) \leq 2 \sqrt{x}$ we get

$$\sum_{k \geq J} H(p_k) \leq 2 \sqrt{c_1} \sum_{k \geq J} e^{-(k-1)/4} = O(\delta).$$

Plugging this into Eq. (80) and using the fact that $Q = O(m \log(\omega^{-1}))$ and $J = O(\log(\delta^{-1}))$ gives

$$\text{Tr}(P) = e^{O(m \log(\omega^{-1}) \log(\delta^{-1}))}$$

which completes the proof of Eq. (72). Here we take $\chi = \text{Tr}(P)$ and $\{|\theta_a\rangle\}$ to be the set of Fock basis states which span the image of $P$, so that $P = \sum_{a=1}^{X} |\theta_a\rangle\langle\theta_a|$. 

Using the fact that $\{x^i : i = 1, 2, \ldots, n\}$ is an orthonormal basis of $\mathbb{C}^n$ we get

$$\hat{N} \equiv \sum_{j=1}^{n} \hat{b}^+_j \hat{b}_j = \sum_{j,f,g=1}^{n} \chi_j^f x_g^f \hat{b}^+_j \hat{b}_j = \sum_{j=1}^{n} \hat{b}^+_j \hat{b}_j \equiv N.$$ 

By construction, $\hat{N}|\theta_a\rangle = k_a|\theta_a\rangle$, where

$$k_a \leq m + Q(J - 1) + \sum_{k \geq J} R_k \leq cm \log(2\omega^{-1}) \log(\delta^{-1})$$

for some universal constant $c > 0$. This implies $N|\theta_a\rangle = k_a|\theta_a\rangle$, as claimed in Eq. (73). Furthermore, $[P, N] = [P, \hat{N}] = 0$ since $P$ and $\hat{N}$ are both diagonal in the Fock basis $\{|\theta\rangle\}$. We also have $[P, H_{imp}] = 0$ which follows from Eqs. (76, 79). $\square$

For future reference, let us summarize properties of $P$ that follow trivially from Corollary 2:

$$[P, H_{imp}] = [P, \sum_{j=1}^{n} \hat{b}^+_j \hat{b}_j] = 0 \quad \text{and} \quad \| \sum_{j=1}^{n} \hat{b}^+_j \hat{b}_j P \| \leq cm \log(2\omega^{-1}) \log(\delta^{-1}).$$

(81)
4. Algorithms and Complexity

In this section we consider the problem of approximating the ground energy of a quantum impurity model. We begin in Sect. 4.1 with some technical tools used in subsequent sections: a decoupling lemma which describes how to identify and decouple canonical bath modes which commute with the impurity, and a truncation lemma which shows that the ground energy can change by at most $\epsilon$ if we take all single-particle energies of $H_0$ below $\epsilon/m$ and round them up to $\epsilon/m$. In Sect. 4.2 we present and analyze our quasipolynomial algorithm for approximating the ground energy of a quantum impurity model (that is, we prove Theorem 1). In Sect. 4.3 we consider the case where the full Hamiltonian $H$ has a constant spectral gap and in this case we give a polynomial time algorithm (proving Theorem 3).

4.1. Bath decoupling and truncation. In this section we present two tools for simplifying quantum impurity problems.

The first tool is a decoupling lemma which is useful when the single-particle spectrum $\{\epsilon_j : j \in [n]\}$ contains degeneracy. We say that a fermi mode $\tilde{b}_j$ is coupled to the impurity if $[\tilde{b}_j, H_{imp}] \neq 0$. The decoupling lemma states that we may choose a set of fermi modes which diagonalize the bath Hamiltonian $H_0$ and such that at most $m$ of the modes with a given single-particle energy $\epsilon_j$ are coupled to the impurity.

**Lemma 3 (Decoupling lemma).** Let $H = H_0 + H_{imp}$ be a quantum impurity model, and write

$$H_0 = \sum_{j=1}^{n} \epsilon_j \tilde{b}_j \tilde{b}_j = \sum_{k} e_k \left( \sum_{j \in Q_k} b_j \tilde{b}_j + \sum_{j \in B_k} \tilde{b}_j b_j \right)$$

where $\{e_k\}$ are the distinct single particle energies and $Q_k \subseteq [n]$ contains all modes with energy $e_k$. We may choose fermion operators $\{\tilde{b}_j : j = 1, \ldots, n\}$ such that $H_0$ is diagonalized as

$$H_0 = \sum_{k} e_k \left( \sum_{i \in A_k} \tilde{b}_i \tilde{b}_i + \sum_{i \in B_k} \tilde{b}_i \tilde{b}_i \right)$$

where $|B_k| \leq m$ for all $k$, and

$$[\tilde{b}_i, H_{imp}] = 0 \quad \text{for all } i \in \bigcup_k A_k.$$  \hspace{1cm} (84)

A particle-number conserving Gaussian unitary $V$ such that $\tilde{b}_j = V^* b_j V$ for all $j \in [n]$ can be computed in $O(n^3)$ time.

**Proof.** Suppose that the operators $\{b_j\}$ in Eq. (82) do not already satisfy the additional constraints in the Lemma. We will show how a Gaussian unitary transformation gives a new set of operators which satisfy these constraints.

Each operator $b_i$ can itself be expressed as a linear combination of the Majorana operators $\{c_1, c_2, \ldots, c_{2n}\}$. For all $i \in Q_k$ we have

$$b_i = \sum_{j=1}^{2n} T^{(k)}_{ij} c_j$$
where \( T^{(k)} \) is a \(|Q_k| \times 2n\) complex matrix. A QR decomposition gives a \(|Q_k| \times |Q_k|\) unitary \( U^{(k)} \) such that \( U^{(k)}T^{(k)} \) is in reduced row echelon form. We may compute \( U^{(k)} \) using \( O(|Q_k|n^2) \) arithmetic operations. Setting

\[
\tilde{b}_j = \sum_{s\in Q_k} U^{(k)}(j) b_s = \sum_{p=1}^{2n} (U^{(k)}T^{(k)})_{jp} c_p \quad j = 1 \ldots, |Q_k| \quad k = 0, 1, 2, \ldots
\]  

we see that the new creation and annihilation operators satisfy the fermion anticommutation relations and that

\[
\sum_{j\in Q_k} \tilde{b}_j^\dagger \tilde{b}_j = \sum_{i\in Q_k} b_i^\dagger b_i
\]

and therefore \( H_0 \) satisfies Eq. (82) with \( b_i \) replaced by \( \tilde{b}_i \). From Eq. (85) we see that the Gaussian unitary \( V \) which maps \( b_j \to \tilde{b}_j \) is associated with a linear transformation of fermion operators given by the block diagonal unitary \( \bigoplus_k U^{(k)} \). The total runtime for computing all blocks of this unitary is \( O(\sum_k |Q_k|n^2) = O(n^3) \).

Now focus on a fixed \( k \), look at Eq. (85) and recall that \( U^{(k)}T^{(k)} \) is in reduced row echelon form. We see that there are at most \( m \) modes in the set \( \{\tilde{b}_j : j \in Q_k\} \) for which the right-hand side of Eq. (85) has a nonzero coefficient for the impurity Majorana modes \( \{c_1, \ldots, c_m\} \). We partition \( Q_k = A_k \cup B_k \) where \( |B_k| \leq m \) indexes these modes. Eq. (84) then follows, using the fact that \( H_{imp} \) acts non-trivially only on the modes \( c_1, \ldots, c_m \) and includes only even weight Majorana monomials. \( \square \)

The second tool is a truncation lemma which bounds the change in the ground energy of \( H \) when we truncate the single particle energies of the bath \( H_0 \) below a given threshold. Let a target precision \( \gamma > 0 \) be given and let \( \Omega \) index the single particle energies of \( H_0 \) which are at most \( \gamma/m \), i.e.,

\[
\Omega = \{ j \in [n] : \epsilon_j \leq \gamma/m \} \quad \Omega^c = [n] \setminus \Omega.
\]

Define a truncated impurity model

\[
H(\gamma) = H_0(\gamma) + H_{imp} \quad H_0(\gamma) = \frac{\gamma}{m} \sum_{j \in \Omega} b_j^\dagger b_j + \sum_{j \in \Omega^c} \epsilon_j b_j^\dagger b_j.
\]  

Here we have set all energies \( \epsilon_j \leq \gamma/m \) to be equal to \( \gamma/m \). Write \( e_{\gamma}(\gamma) \) for the ground energy of \( H(\gamma) \).

**Lemma 4** (Truncation lemma).

\[
|e_{\epsilon} - e_{\gamma}(\gamma)| \leq \gamma.
\]

**Proof.** First define another Hamiltonian

\[
\hat{H}(\gamma) = \sum_{j \in \Omega^c} \epsilon_j b_j^\dagger b_j + H_{imp}
\]
and let its ground energy be $\hat{e}_g(\gamma)$. We have the operator inequality $\hat{H}(\gamma) \leq H \leq H(\gamma)$ and thus $\hat{e}_g(\gamma) \leq e_g \leq e_g(\gamma)$. To prove the proposition we now show that $e_g(\gamma) - \hat{e}_g(\gamma) \leq \gamma$. Let $|\theta\rangle$ be a ground state of $\hat{H}(\gamma)$ such that

$$\langle \theta | \sum_{j \in \Omega} b_j^\dagger b_j | \theta \rangle \leq m.$$

It is always possible to choose such a ground state since all but $m$ of the modes in $\Omega$ can be decoupled from the impurity. That is, Lemma 3 implies that we may define new fermi modes $\tilde{b}_j$ such that

$$\sum_{j \in \Omega} b_j^\dagger b_j = \sum_{j \in A} \tilde{b}_j^\dagger \tilde{b}_j + \sum_{j \in B} \tilde{b}_j^\dagger \tilde{b}_j$$

and $[\tilde{b}_j, H_{imp}] = [\tilde{b}_j, \hat{H}(\gamma)] = 0$ for all $j \in A$ and $|B| \leq m$. This implies we may choose a ground state $|\theta\rangle$ of $\hat{H}(\gamma)$ such that $\tilde{b}_j^\dagger \tilde{b}_j |\theta\rangle = 0$ for all $j \in A$ and thus

$$\langle \theta | \sum_{j \in \Omega} b_j^\dagger b_j | \theta \rangle = \langle \theta | \sum_{j \in B} \tilde{b}_j^\dagger \tilde{b}_j | \theta \rangle \leq m.$$

Now

$$\hat{e}_g(\gamma) = \langle \theta | H(\gamma) | \theta \rangle + \langle \theta | \hat{H}(\gamma) - H(\gamma) | \theta \rangle \geq e_g(\gamma) - |\langle \theta | \hat{H}(\gamma) - H(\gamma) | \theta \rangle|.$$

Therefore

$$e_g(\gamma) - \hat{e}_g(\gamma) \leq |\langle \theta | \hat{H}(\gamma) - H(\gamma) | \theta \rangle| = \langle \theta | \sum_{j \in \Omega} \frac{\gamma}{m} b_j^\dagger b_j | \theta \rangle \leq \gamma.$$

\[\square\]

4.2. Quasipolynomial algorithm for general impurity models. In this section we describe the quasipolynomial algorithm for approximating the ground energy and prove Theorem 1, restated here for convenience.

Theorem 1 (Quasipolynomial algorithm). There exists a classical algorithm which takes as input a quantum impurity model $H$, a target precision $\gamma \in (0, 1/2]$, and outputs an estimate $E$ such that $|E - e_g| \leq \gamma$. The algorithm has runtime

$$O(n^3) \exp \left[ O(m \log^3 (m \gamma^{-1})) \right].$$

We begin by introducing some additional notation used in this section. Define an operator

$$\mathcal{N} = \sum_{j=1}^{n} b_j^\dagger b_j$$

which counts the number of excitations of the bath. For any $s \geq 0$ define $\mathcal{W}(s)$ to be the subspace spanned by all eigenvectors of $\mathcal{N}$ with eigenvalue at most $s$. Corollary 2 states
that (at least one) ground state $\psi$ of an impurity model $H$ is approximated to precision $\delta$ by a state in $W(s)$ whenever
\[ s \geq cm \log(2\omega^{-1}) \log(\delta^{-1}) \]
for some universal constant $c > 0$. In this section we are interested in approximating the ground energy rather than the ground state itself. We use Corollary 2 and Lemma 4 to prove the following lemma.

**Lemma 5.** Let $\gamma \in (0, 1/2]$ be a precision parameter. We have
\[ e_g \leq \min_{\alpha \in W(s)} \langle \alpha | H | \alpha \rangle \leq e_g + \gamma \]
whenever
\[ s \geq cm \log^2(m\gamma^{-1}) \]
where $c > 0$ is a universal constant.

**Proof.** The lower bound in Eq. (87) is trivial; below we prove the upper bound. Recall that we write $\omega$ for the spectral gap of the bath Hamiltonian $H_0$, that is, all nonzero single-particle excitation energies $\epsilon_j$ are in the interval $[\omega, 1]$. Let $\gamma > 0$ be the desired precision.

As a first step we give a reduction to the special case where $\omega = \gamma/m$. The reduction is based on the truncation lemma (Lemma 4). Let $H(\gamma)$ be given as in Eq. (86). By definition the bath Hamiltonian $H_0(\gamma)$ has spectral gap $\omega = \gamma/m$. We have the operator inequality $H \leq H(\gamma)$ and therefore
\[ \min_{\alpha \in W(s)} \langle \alpha | H | \alpha \rangle \leq \min_{\alpha \in W(s)} \langle \alpha | H(\gamma) | \alpha \rangle. \]  
(89)

Suppose that Lemma 5 holds for precision $\gamma$ and Hamiltonian $H(\gamma)$. Then, using Lemma 4 and Eq. (89) we get
\[ \min_{\alpha \in W(s)} \langle \alpha | H | \alpha \rangle \leq e_g(\gamma) + \gamma \leq e_g + 2\gamma. \]
(90)
whenever
\[ s \geq c'm \log^2(m/(2\gamma)) \geq cm \log^2(m\gamma^{-1}) \]
(91)
where $c' > 0$ is another universal constant. Eqs. (90, 91) complete the reduction; they are Eqs. (87, 88) for the original Hamiltonian $H$, precision $2\gamma$, and constant $c'$. Thus we have shown Lemma 5 follows from its special case where $\omega = \gamma/m$.

To complete the proof, we now establish the lemma assuming $\omega = \gamma/m$. Fix some $\delta \in (0, 1/2]$ and let $\psi \in H_n$ be a normalized ground state of $H$ from Corollary 2. Let $P$ be the projector defined in Eq. (74). Corollary 2 states that $[H_{imp}, P] = 0$, and that $\|\psi - \phi\| \leq \delta$ with $P|\phi\rangle = |\phi\rangle$, which implies $\langle \psi | I - P | \psi \rangle \leq \delta^2$. Using these facts we get
\[
\left| e_g - \frac{\langle \psi | PHP | \psi \rangle}{\langle \psi | P | \psi \rangle} \right| = \frac{1}{\langle \psi | P | \psi \rangle} \left| \langle \psi | (I - P)HP | \psi \rangle \right|
\leq \frac{1}{\langle \psi | P | \psi \rangle} \left| \langle \psi | (I - P)H_0P | \psi \rangle \right|
\leq \sqrt{\langle \psi | (I - P) | \psi \rangle} \langle \psi | P | \psi \rangle \|H_0P\|
\leq 2\delta \|H_0P\| \]
(92)
where in the last line we used \( \delta \leq \frac{1}{\sqrt{2}} \). Now \( H_0 \leq \mathcal{N} \) and, since both operators are diagonal over the same basis we also have \( H_0^2 \leq \mathcal{N}^2 \). Using this fact and Eq. (81) we get

\[
\|H_0 P\| \leq \|\mathcal{N} P\| \leq cm \log(2\omega^{-1}) \log(\delta^{-1}) = cm \log(2m\gamma^{-1}) \log(\delta^{-1})
\]  

(93)

for some constant \( c > 0 \). In the last equality we substituted \( \omega = \gamma/m \). Since \( \gamma \leq 1/2 \) and \( m \geq 1 \) we have \( \log(2m\gamma^{-1}) \leq O(1) \cdot \log(m\gamma^{-1}) \) and therefore

\[
\|H_0 P\| \leq \|\mathcal{N} P\| \leq c_1 m \log(m\gamma^{-1}) \log(\delta^{-1})
\]  

(94)

where \( c_1 \) is another universal constant. Combining Eqs. (92, 94) we get

\[
\left| e_g - \frac{\langle \psi | PHP | \psi \rangle}{\langle \psi | P | \psi \rangle} \right| \leq 2\delta c_1 m \log(m\gamma^{-1}) \log(\delta^{-1})
\]  

(95)

Now we choose \( \delta \) such that the right hand side is at most \( \gamma \). It suffices to take

\[
\delta = \frac{\gamma}{C m \log^2(m\gamma^{-1})}
\]  

(96)

where \( C \) is any universal constant satisfying \( 2c_1 C^{-1}(\log(C) + 3) \leq 1 \). Indeed, with this choice we have

\[
2\delta c_1 m \log(m\gamma^{-1}) \log(\delta^{-1}) = \frac{2c_1}{C} \left[ \frac{\log(C)}{\log(m\gamma^{-1})} + 1 + 2 \frac{\log(\log(m\gamma^{-1}))}{\log(m\gamma^{-1})} \right] \leq \gamma
\]  

(97)

where we used the fact that the quantity in square parentheses is at most \( \log(C) + 3 \). Thus

\[
\frac{\langle \psi | PHP | \psi \rangle}{\langle \psi | P | \psi \rangle} \leq e_g + \gamma
\]  

(98)

From Eqs. (81, 94) we have \([P, \mathcal{N}] = 0\) and

\[
\|\mathcal{N} P\| \leq c_1 m \log(m\gamma^{-1}) \log(\delta^{-1}) \leq \gamma/2\delta = (C/2)m \log^2(m\gamma^{-1}).
\]

where in the second inequality we used Eq. (97) and in the last inequality we used Eq. (96). This implies that the image of \( P \) is contained in the subspace \( \mathcal{W}(s) \) whenever

\[
s \geq (C/2)m \log^2(m\gamma^{-1}).
\]  

(99)

Thus, for all \( s \) satisfying Eq. (99) we have

\[
\min_{\alpha \in \mathcal{W}(s)} \langle \alpha | H | \alpha \rangle \leq \frac{\langle \psi | PHP | \psi \rangle}{\langle \psi | P | \psi \rangle} \leq e_g + \gamma
\]

where in the second inequality we used Eq. (98). \( \square \)
We now define a deformed impurity model. Let $\gamma \in (0, 1/2]$ be a precision parameter, let $s^* = \lceil cm \log^2(m\gamma^{-1}) \rceil$ be the smallest integer greater than or equal to the right hand side of Eq. (88) and consider a set of grid points

$$G = \{x \gamma/s^* : x \in \{1, 2, \ldots\}\}.$$  

(100)

For each $j$ let $\epsilon'_j$ be the smallest element of $G$ which is at least $\epsilon_j$, so that

$$\epsilon_j \leq \epsilon'_j \leq \epsilon_j + \gamma/s^* \quad j = 1, 2, \ldots, n.$$  

(101)

Define deformed Hamiltonians

$$H'_0 = \sum_{j=1}^{n} \epsilon'_j b_j^\dagger b_j, \quad \text{and} \quad H' = H'_0 + H_{imp}.$$  

Finally, define

$$e^*_g = \min_{\phi \in \mathcal{W}(s^*)} \langle \phi | H'| \phi \rangle.$$  

(102)

The following lemma shows that $e^*_g$ is a good approximation to $e_g$. Our algorithm for approximating $e_g$ is based on computing $e^*_g$.

**Lemma 6.**

$$|e_g - e^*_g| \leq 2\gamma.$$  

**Proof.** Applying Lemma 5 gives

$$|e_g - \min_{\phi \in \mathcal{W}(s^*)} \langle \phi | H| \phi \rangle| \leq \gamma.$$  

Therefore

$$|e_g - e^*_g| \leq \gamma + \left| \min_{\phi \in \mathcal{W}(s^*)} \langle \phi | H'| \phi \rangle - \min_{\phi \in \mathcal{W}(s^*)} \langle \phi | H| \phi \rangle \right| \leq \gamma + \|(H' - H)|_{\mathcal{W}(s^*)}\|$$  

(103)

(104)

where in the last line we used Weyl’s inequality. Here we use the notation $M|_{\mathcal{S}}$ to denote the restriction of an operator $M$ to a subspace $\mathcal{S}$. Now

$$H' - H = \sum_{j=1}^{n} (\epsilon'_j - \epsilon_j) b_j^\dagger b_j$$

and using Eq. (101) we arrive at

$$0 \leq H' - H \leq \frac{\gamma}{s^*} \sum_{j=1}^{n} b_j^\dagger b_j.$$  

Thus

$$\|(H' - H)|_{\mathcal{W}(s^*)}\| \leq \frac{\gamma}{s^*} \left\| \left( \sum_{j=1}^{n} b_j^\dagger b_j \right) \right\|_{\mathcal{W}(s^*)} \leq \gamma,$$  

(105)

where in the last line we used the definition of $\mathcal{W}(s^*)$. Plugging this into Eq. (104) completes the proof. $\square$
Thus we have shown that to approximate $\epsilon_R$ it suffices to consider the deformed impurity model. Why is this useful to us? The total number of distinct single-particle energies $\epsilon_j'$ is at most $1 + |G \cap [0, 1]| \leq 1 + s^* / \gamma$, which does not depend on $n$. Since there are $n$ modes in total, we see that on average a single-particle energy of the deformed bath $H_0'$ has degeneracy linear in $n$. Because of this massive degeneracy, we may use the decoupling lemma to show that many of the degrees of freedom (modes) can be decoupled from the impurity.

Applying Lemma 3 to the deformed impurity model $H'$ we get fermion operators $\{\tilde{b}_j : j = 1, \ldots, n\}$ and subsets $A_k, B_k \subseteq [n]$ such that

$$H_0' = \sum_{k=1,2,\ldots} \frac{k\gamma}{s^*} \left( \sum_{i \in A_k} \tilde{b}_i^\dagger \tilde{b}_i + \sum_{i \in B_k} \tilde{b}_i^\dagger \tilde{b}_i \right)$$

(106)

such that $|B_k| \leq m$ and the modes in $\cup_k A_k$ are decoupled from the impurity, that is,

$$[\tilde{b}_j, H_{imp}] = 0 \quad \text{whenever} \quad \tilde{b}_j \in \cup_k A_k. \quad (107)$$

For ease of notation, let us order the modes so that the decoupled ones appear first

$$\cup_k A_k = \{1, 2, \ldots, N\} \quad \cup_k B_k = \{N + 1, N + 2, \ldots, n\}$$

Note that the total number of coupled modes is upper bounded by $m$ times the number of distinct single particle energy levels $\epsilon_j'$, that is,

$$n - N \leq m(1 + |G \cap [0, 1]|) \leq m(1 + s^* / \gamma) \leq \frac{2ms^*}{\gamma}. \quad (108)$$

For each $\tilde{z} \in \{0, 1\}^n$ define a Fock basis state $|\tilde{z}\rangle$ with respect to the modes $\{\tilde{b}_j\}$, i.e.,

$$\tilde{b}_j^\dagger \tilde{b}_j |\tilde{z}\rangle = z_j |\tilde{z}\rangle \quad j = 1, 2, \ldots, n. \quad (109)$$

Note that $|\tilde{z}\rangle$ is an eigenstate of the operator $\sum_j \tilde{b}_j^\dagger \tilde{b}_j$ with eigenvalue $\sum_{j=1}^n z_j$. Lemma 3 states that the decoupling transformation preserves particle number, that is,

$$N = \sum_{j=1}^n \tilde{b}_j^\dagger \tilde{b}_j = \sum_{j=1}^n \tilde{b}_j^\dagger \tilde{b}_j. \quad (110)$$

By definition, the subspace $W(s^*)$ is spanned by all eigenstates of the number operator Eq. (110) with eigenvalues at most $s^*$. Therefore

$$W(s^*) = \text{span} \left\{ |\tilde{z}\rangle : \sum_{i=1}^n z_i \leq s^* \right\}. \quad (110)$$

Define a subspace

$$\mathcal{V} = \text{span} \left\{ |\tilde{z}\rangle : \sum_{i=1}^n z_i \leq s^* \quad \text{and} \quad z_1 = z_2 = \cdots = z_N = 0 \right\} \quad (111)$$

spanned by basis vectors where the decoupled modes are unoccupied. We now show that the minimization in Eq. (102) can be restricted to the subspace $\mathcal{V}$. 

Lemma 7.
\[ e_g^* = \min_{\phi \in \mathcal{V}} \langle \phi | H' | \phi \rangle. \] (112)

Proof. Eqs. (106, 107) imply \[ [\tilde{b}_j^+, \tilde{b}_j, H'] = 0 \] for all \( j \in \{1, 2, \ldots, N\} \) and therefore
\[ \langle \tilde{z} | H' | \tilde{y} \rangle = 0 \quad \text{whenever} \quad y_i \neq z_i \quad \text{for some} \quad i \in \{1, 2, \ldots, N\}. \]
Thus the restriction \( H'|_{\mathcal{W}(s^*)} \) is block diagonal in the basis \( \{|\tilde{z}\rangle : z \in \{0, 1\}^n\} \) with a block for each configuration \( z_1 z_2 \ldots z_N \) of the decoupled modes. The smallest eigenvalue \( e_g^* \) of \( H'|_{\mathcal{W}(s^*)} \) is the smallest eigenvalue of one of the blocks. In particular, for some \( |\phi\rangle \) and \( x \in \{0, 1\}^N \) we have
\[ e_g^* = \langle \phi | H' | \phi \rangle \quad \text{and} \quad \tilde{b}_j^+ \tilde{b}_j |\phi\rangle = x_j |\phi\rangle \quad j = 1, 2, \ldots, N. \]
Now let \( |\alpha\rangle = \tilde{b}_1^{s_1} \tilde{b}_2^{s_2} \ldots \tilde{b}_N^{s_N} |\phi\rangle \) and note that \( \alpha \in \mathcal{V} \). Applying Lemma 3 we get
\[ \langle \alpha | H_0' | \alpha \rangle \leq \langle \phi | H_0' | \phi \rangle \quad \text{and} \quad \langle \alpha | H_{imp} | \alpha \rangle = \langle \phi | H_{imp} | \phi \rangle \]
and therefore \( \langle \alpha | H' | \alpha \rangle \leq \langle \phi | H' | \phi \rangle \). Note that equality must hold since \( \phi \) minimizes the energy of \( H' \) in \( \mathcal{W}(s^*) \). We have shown there exists \( \alpha \in \mathcal{V} \) with \( e_g^* = \langle \alpha | H' | \alpha \rangle \), which completes the proof. \( \square \)

Using Eq. (111) gives
\[ \dim(\mathcal{V}) \leq \sum_{k=0}^{s^*} \binom{n-N}{k}. \]
We now show that
\[ \dim(\mathcal{V}) \leq e^{O(m \log^3(m \gamma^{-1}))}. \] (113)
To arrive at Eq. (113), suppose first that \( s^* \leq \frac{n-N}{2} \). Then \( \sum_{k=0}^{s^*} \binom{n-N}{k} \leq (s^* + 1)(\frac{n-N}{s^*}) \)
and hence
\[ \dim(\mathcal{V}) \leq (s^* + 1) \left( e^{\frac{n-N}{s^*}} \right)^{s^*} \leq (s^* + 1) \left( \frac{2em}{\gamma} \right)^{s^*} = e^{O(m \log^3(m \gamma^{-1}))}. \] (114)
where we used the bound \( \binom{n}{k} \leq (le/k)^k \) where \( e = \exp(1) \). On the other hand if \( s^* > \frac{n-N}{2} \) then we get a slightly stronger bound
\[ \dim(\mathcal{V}) \leq \sum_{k=0}^{s^*} \binom{n-N}{k} \leq 2^{n-N} \leq 2^{2s^*} \leq e^{O(m \log^2(m \gamma^{-1}))}. \]
This establishes Eq. (113).

Let \( D \equiv \dim(\mathcal{V}) \). We claim that the righthand side of Eq. (112) can be computed in time \( O(2^n n^3 D^2 + D^3) \). Indeed Eq. (111) gives an orthonormal set of Gaussian states \( \Phi = \{\phi_1, \ldots, \phi_D\} \) that spans \( \mathcal{V} \). By construction, the deformed bath Hamiltonian is diagonal in this basis and one can compute a matrix element \( \langle \phi_j | H_0' | \phi_j \rangle \) in time \( O(n) \) by summing up energies of all excitations present in \( \phi_j \). Thus one can compute the matrix of \( H_0' \) in the basis \( \Phi \) in time \( O(nD) \). Consider now the impurity Hamiltonian
\( H_{\text{imp}} \). By construction, \( H_{\text{imp}} \) is a linear combination of \( O(2^m) \) Majorana monomials \( c(x) \). Using the generalized Wick’s theorem Eq. (26) one can compute a single matrix element \( \langle \phi_i | c(x) | \phi_j \rangle \) in time \( O(n^3) \). Thus one can compute the full matrix of \( H_{\text{imp}} \) in the basis \( \Phi \) in time \( O(2^m n^3 D^2) \). Once the matrices of \( H_0^i \) and \( H_{\text{imp}} \) in the basis \( \Phi \) are computed, one can calculate \( e_g^\star \) using exact diagonalization in time \( O(D^3) \). Recall that \( |e_g - e_g^\star| \leq 2\gamma \) (to get rid of the factor of 2 we may rescale the precision parameter \( \gamma \) → 2\gamma without altering the asymptotic runtime of the algorithm). This completes the proof of Theorem 1.

Remark. The above algorithm can be used to produce a low energy state of \( H \), the original (not deformed) impurity model. Indeed, in the last step of the algorithm, one may use an exact diagonalization routine which, along with the eigenvalue \( \gamma \), may use an exact diagonalization routine which, along with the eigenvalue \( \gamma \), computes a state \( \alpha \in \mathcal{V} \subseteq W(s^\star) \) satisfying \( e_g^\star = \langle \alpha | H' | \alpha \rangle \). In this case we have

\[
e_g^\star - \langle \alpha | H | \alpha \rangle = \langle \alpha | H' | \alpha \rangle - \langle \alpha | H | \alpha \rangle \leq \| (H' - H) |_{W(s^\star)} \| \leq \gamma
\]

where we used Eq. (105). Combining this with the fact that \( |e_g - e_g^\star| \leq 2\gamma \), we see that the computed state \( |\alpha\rangle \) satisfies

\[
|e_g - \langle \alpha | H | \alpha \rangle| \leq 3\gamma.
\]

4.3. Efficient algorithm for gapped impurity models. In this section we prove Theorem 3, restated here for convenience.

**Theorem 3.** Suppose the impurity has size \( m = O(1) \). Suppose the full Hamiltonian \( H \) has a non-degenerate ground state and a constant energy gap above the ground state. Then there exists a classical algorithm that approximates the ground energy \( e_g \) within a given precision \( \delta \) in time \( \text{poly}(n, \delta^{-1}) \).

**Proof.** Let \( e^1, e^2, \ldots, e^{2n} \) be the standard basis of \( \mathbb{R}^{2n} \). Let \( h \) be the \( 2n \times 2n \) matrix defined in Eq. (3). Define a nested sequence of linear subspaces \( \mathcal{L}_1 \subseteq \mathcal{L}_2 \subseteq \cdots \subseteq \mathcal{L}_v \subseteq \mathbb{R}^{2n} \) such that

\[
\mathcal{L}_1 = \text{span}(e^1, e^2, \ldots, e^m) \quad \text{and} \quad \mathcal{L}_j = \text{span}(\mathcal{L}_1, h\mathcal{L}_1, \ldots, h^{j-1}\mathcal{L}_1)
\]

for \( j \geq 2 \). We choose \( v \) as the smallest integer such that \( \mathcal{L}_{v+1} = \mathcal{L}_v \). Obviously, \( v = O(n) \). Let \( L = \text{dim} (\mathcal{L}_v) \). By construction, \( \mathcal{L}_v \) is \( h \)-invariant. Define a subspace

\[
\mathcal{K}_j = \mathcal{L}_j \cap \mathcal{L}_{j-1}^\perp.
\]

Let us agree that \( \mathcal{L}_0 = 0 \), so that \( \mathcal{K}_1 = \mathcal{L}_1 \). We get a direct sum decomposition

\[
\mathbb{R}^{2n} = \mathcal{K}_1 \oplus \mathcal{K}_2 \oplus \cdots \oplus \mathcal{K}_v \oplus \mathcal{L}_v^\perp.
\]

Note that \( h \) is block-tridiagonal with respect to this decomposition, that is, \( \langle \alpha | h | \beta \rangle = 0 \) whenever \( \alpha \in \mathcal{K}_i, \beta \in \mathcal{K}_j \), and \( |i - j| \geq 2 \). Indeed, assume wlog that \( i \geq j + 2 \). Then

\[
h|\beta\rangle \in h\mathcal{K}_j \subseteq h\mathcal{L}_j \subseteq \mathcal{L}_{j+1} \subseteq \mathcal{L}_{i-1}
\]

whereas \( |\alpha\rangle \in \mathcal{K}_i \subseteq \mathcal{L}_{i-1}^\perp \). Furthermore,

\[
\text{dim} (\mathcal{K}_j) = \text{dim} (\mathcal{L}_j) - \text{dim} (\mathcal{L}_{j-1}) \leq m
\]

since \( \mathcal{L}_j \) is spanned by \( \mathcal{L}_{j-1} \) and \( h^{j-1}\mathcal{L}_1 \).
Choose an orthonormal basis $f^1, f^2, \ldots, f^{2n} \in \mathbb{R}^{2n}$ such that the first $\dim(K_1)$ basis vectors span $K_1$, the next $\dim(K_2)$ basis vectors span $K_2$ and so on. The last $2n - \dim(L_v)$ basis vectors span $L_v^\perp$. Define a new set of Majorana operators

$$\tilde{c}_p = \sum_{q=1}^{2n} (f^p)_q c_q, \quad p = 1, \ldots, 2n.$$  \hspace{1cm} (116)

Here $(f^p)_q$ is the $q$-th component of $f^p$. The operators $\tilde{c}_p$ obey the same commutation rules as $c_p$. By construction, $\tilde{c}_p = c_p$ for $1 \leq p \leq m$ and thus $H_{imp}$ belongs to the algebra generated by $\tilde{c}_1, \ldots, \tilde{c}_m$. Transforming $h$ to the new basis we find that

$$h = \begin{bmatrix} h' & 0 \\ 0 & h'' \end{bmatrix},$$  \hspace{1cm} (117)

where the two blocks have dimension $L$ and $2n - L$ respectively. Moreover, $h'$ is block-tridiagonal with non-zero matrix elements only between blocks $K_i, K_j$ with $|i - j| \leq 1$. We conclude that

$$H = H_{imp} + H_A + H_B, \quad H_A = \frac{i}{4} \sum_{p,q=1}^{L} h'_{p,q} \tilde{c}_p \tilde{c}_q, \quad H_B = \frac{i}{4} \sum_{p,q=L+1}^{2n} h''_{p,q} \tilde{c}_p \tilde{c}_q.$$  \hspace{1cm} (118)

For simplicity, here we ignore the constant energy shift in Eq. (3). The terms $H_{imp} + H_A$ and $H_B$ act on disjoint sets of modes and the ground energy of $H$ is the sum of their ground energies. Since $H_B$ is quadratic its ground energy is $-\|h''\|_1/4$, which is easily computed from the singular value decomposition of $h''$. Thus we can concentrate on $H_{imp} + H_A$ which acts on modes $\tilde{c}_1, \ldots, \tilde{c}_L$. Without loss of generality we shall assume $L$ is even in the following; if it is not even we may simply view $H_{imp} + H_A$ as acting on modes $\tilde{c}_1, \ldots, \tilde{c}_L$ in addition to one auxiliary Majorana mode. We can map $H_{imp} + H_A$ to a Hamiltonian describing a 1D chain of qubits using the standard Jordan–Wigner transformation:

$$\tilde{c}_1 = X_1, \quad \tilde{c}_2 = Y_1,$$

and

$$\tilde{c}_{2a-1} = Z_1 \cdots Z_{a-1} X_a \quad \text{and} \quad \tilde{c}_{2a} = Z_1 \cdots Z_{a-1} Y_a$$

for $a \geq 2$. Here $X_a, Y_a, Z_a$ are the Pauli operators on the $a$-th qubit. Since we have $L$ Majorana modes, the chain consists of $L/2$ qubits. We may coarse-grain the chain such that the first $m$ qubits form the first site, the next $m$ qubits form the second site, and so on (the last qudit may consist of $< m$ qubits). Since $h'$ is block tridiagonal with block size upper bounded as $\dim(K_j) \leq m$, we have

$$h'_{ij} = 0 \quad \text{whenever} \quad |i - j| \geq 2m.$$  

This block tridiagonal structure implies that after the Jordan–Wigner transformation the Hamiltonian $H_{imp} + H_A$ describes a 1D chain of qubits with nearest-neighbor interactions. Each qudit has dimension at most

$$d = 2^m = O(1).$$

The chain has length $v = O(n)$. Since all of the above transformations are unitary, they preserve eigenvalues. Thus a gapped quantum impurity model can be efficiently mapped to a gapped 1D chain of qudits. One can approximate the ground state energy of the latter within error $\delta$ in time $\text{poly}(n, \delta^{-1})$ using MPS-based algorithms, see Ref. [19].
5. Simplified Practical Algorithm

In this section we describe a variational algorithm that minimizes the energy of a quantum impurity Hamiltonian over low-rank superpositions of Gaussian states. We benchmark the method using the single impurity Anderson model [1].

Consider a system of \( n \) fermi modes and a Hamiltonian composed of arbitrary quadratic and quartic Majorana monomials:

\[
H = H_0 + H_{imp},
\]

\[
H_0 = i \sum_{1 \leq p < q \leq 2n} A_{pq} c_p c_q,
\]

\[
H_{imp} = \sum_{1 \leq p < q < r < s \leq m} U_{pqrs} c_p c_q c_r c_s.
\]

Here \( A_{pq} \) and \( U_{pqrs} \) are some real coefficients. We shall extend the range of all sums over Majorana modes to the interval \([1, 2n]\) assuming that \( U_{pqrs} = 0 \) unless \( 1 \leq p < q < r < s \leq m \). Since the Hamiltonian \( H \) commutes with the parity operator \( P \), see Eq. (19), we can minimize the energy of \( H \) in the even and the odd subspaces separately. Equivalently, one can minimize the energy of \( H \) and \( c_1 H c_1 \) within the even subspace. Since both minimizations are exactly the same, below we consider only the even subspace.

Our variational algorithm depends on an integer \( \chi \geq 1 \) that we call a rank. Let

\[
\Phi = (\phi_1, \phi_2, \ldots, \phi_\chi)
\]

be a tuple of \( \chi \) even Gaussian states \( \phi_a \in G_n \) with covariance matrices \( M_a \). The states \( \phi_a \) may or may not be pairwise orthogonal. The algorithm works by minimizing an objective function \( E(M_1, \ldots, M_\chi) \) defined as the smallest eigenvalue of \( H \) restricted to the linear subspace spanned by states \( \phi_1, \ldots, \phi_\chi \):

\[
E(M_1, \ldots, M_\chi) = \min_{\psi \in \text{span}(\Phi)} \frac{\langle \psi | H | \psi \rangle}{\langle \psi | \psi \rangle}.
\]

Here \( \text{span}(\Phi) \equiv \text{span}(\phi_1, \ldots, \phi_\chi) \). Note that \( \text{span}(\Phi) \) is uniquely determined by the covariance matrices \( M_1, \ldots, M_\chi \).

We shall parameterize the covariance matrix of \( \phi_a \) by a rotation \( R_a \in SO(2n) \) such that

\[
M_a = R_a M_{\text{vac}} R_a^T.
\]

Here

\[
M_{\text{vac}} = \bigoplus_{j=1}^{n} \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix}
\]

is the covariance matrix of the vacuum state \(|0^n\rangle\), see Eq. (18). Thus we have to minimize the objective function Eq. (122) over the group

\[
SO(2n) \times \cdots \times SO(2n),
\]

where the direct product contains \( \chi \) factors.
5.1. Rank-1 algorithm. Let us start from the simplest case $\chi = 1$, i.e. minimizing the energy of $H$ over all Gaussian states. This corresponds to a generalized Hartree-Fock method proposed recently by Kraus and Cirac [18] for simulation of interacting fermions on a lattice. Let $M \equiv M_1$. Applying Wick’s theorem Eq. (21) one gets

$$E(M) = \frac{1}{2} \text{Tr}(AM) - \sum_{p < q < r < s} U_{pqrs} \text{Pf}(M[p, q, r, s]).$$

(124)

We initialize $M = R M_{\text{vac}} R^T$, where $R \in SO(2n)$ is chosen at random. The energy $E(M)$ is then minimized by a greedy random walk algorithm. Each step of the walk generates a random rotation $R \in SO(2n)$ such that $\|R - I\| \leq \theta$ for some specified angle $\theta$. A step is deemed successful if it decreases the value of the objective function, $E(RMR^T) < E(M)$. In this case $M$ is replaced by $RMR^T$. Otherwise $M$ remains unchanged. The angle $\theta$ is adjusted by keeping track of the fraction of successful steps $f$. We fix some threshold value $f_0$ and adjust the angle as $\theta \leftarrow \theta(1 + \epsilon)$ if $f \geq f_0$ and $\theta \leftarrow \theta(1 - \epsilon)$ if $f < f_0$. Here $\epsilon$ is a small constant. We empirically found that $\epsilon = 0.2$ and $f_0 = 0.1$ works reasonably well.

5.2. Rank-2 algorithm. Define a $2 \times 2$ Gram matrix $G$ such that $G_{a,b} = \langle \phi_a | \phi_b \rangle$. We can always choose the relative phase of $\phi_1$ and $\phi_2$ such that $G$ is a real matrix. Then

$$G = \begin{bmatrix} 1 & g \\ g & 1 \end{bmatrix}, \quad \text{where} \quad g = \langle \phi_1 | \phi_2 \rangle = 2^{-n/2} \det(M_1 + M_2)^{1/4}. \quad (125)$$

Here we used Eq. (22). Using the generalized Wick’s theorem Eq. (27) one gets

$$\langle \phi_a | H_0 | \phi_a \rangle = \frac{1}{2} \text{Tr}(AM_a)$$

(126)

and

$$\langle \phi_2 | H_0 | \phi_1 \rangle = \frac{g}{2} \text{Tr}(A\Delta),$$

(127)

where

$$\Delta = (-2I + iM_1 - iM_2)(M_1 + M_2)^{-1}.$$ 

Using Eqs. (21, 27) again one gets

$$\langle \phi_a | H_{\text{imp}} | \phi_a \rangle = -\sum_{p < q < r < s} U_{pqrs} \cdot \text{Pf}(M_a[p, q, r, s]),$$

(128)

$$\langle \phi_2 | H_{\text{imp}} | \phi_1 \rangle = -g \sum_{p < q < r < s} U_{pqrs} \text{Pf}(\Delta[p, q, r, s]).$$

(129)

Let $F_0$ and $F_{\text{imp}}$ be $2 \times 2$ hermitian operators with matrix elements

$$\langle a | F_0 | b \rangle = \langle \phi_a | H_0 | \phi_b \rangle \quad \text{and} \quad \langle a | F_{\text{imp}} | b \rangle = \langle \phi_a | H_{\text{imp}} | \phi_b \rangle.$$ 

(130)

Here $a, b = 1, 2$. Standard linear algebra implies that the objective function $E(M_1, M_2)$ from Eq. (122) coincides with the minimum eigenvalue of a $2 \times 2$ matrix

$$G^{-1/2}(F_0 + F_{\text{imp}})G^{-1/2}. $$
Equivalently, $E(M_1, M_2)$ is the minimum eigenvalue of a generalized eigenvalue problem \((F_0 + F_{\text{imp}})\psi = \lambda G \psi\). Thus the above formulas allow one to compute $E(M_1, M_2)$ in time $O(n^3)$. The most time consuming steps are clearly computing the inverse and the determinant of $M_1 + M_2$. We then minimize $E(M_1, M_2)$ over $M_1, M_2$ using the same greedy random walk algorithm as in the rank-1 case. The only difference is that at each step we decide whether to rotate $M_1$ or $M_2$ at random.

5.3. Arbitrary rank. Suppose now that $\chi \geq 3$. Let $\phi_0 \in G_n$ be some fixed reference state used to compute inner products, see Sect. 2.4. We chose $\phi_0$ as a ground state of $H_0$, but it could be an arbitrary Gaussian state. For each $a = 1, \ldots, \chi$ define

$$g_a = \langle \phi_0 | \phi_a \rangle. \quad (131)$$

We can always choose the overall phase of $\phi_a$ such that $g_a$ are real and $g_a \geq 0$. Then Eq. (22) implies

$$g_a = 2^{-n/2} \det (M_0 + M_a)^{1/4}, \quad (132)$$

where $M_0$ is the covariance matrix of the reference state. Define a Gram matrix $G$ with matrix elements $G_{a,b} = \langle \phi_a | \phi_b \rangle$, where $1 \leq a, b \leq \chi$. By normalization, one has $G_{a,a} = 1$. From Eq. (24) one gets

$$G_{b,a} = \frac{2^n g_a g_b}{\text{Pf}(\Delta^{a,b} + M_0)} \quad (133)$$

where

$$\Delta^{a,b} = (-2I + i M_a - i M_b)(M_a + M_b)^{-1}. \quad (132)$$

Note that $\Delta^{a,a} = M_a$ and $\Delta^{b,a} = (\Delta^{a,b})^*$. Using the generalized Wick’s theorem Eq. (27) one gets

$$\langle \phi_b | H_0 | \phi_a \rangle = \frac{G_{b,a}}{2} \text{Tr}(A \Delta^{a,b}) \quad (134)$$

and

$$\langle \phi_b | H_{\text{imp}} | \phi_a \rangle = -G_{b,a} \sum_{p < q < r < s} U_{pqr} \text{Pf} \left( \Delta^{a,b} [p, q, r, s] \right) \quad (135)$$

for all $1 \leq a, b \leq \chi$. Now we can compute $E(M_1, \ldots, M_\chi)$ by solving a generalized eigenvalue problem \((F_0 + F_{\text{imp}})\psi = \lambda G \psi\), where now $F_0$ and $F_{\text{imp}}$ are $\chi \times \chi$ hermitian operators defined by Eq. (130) and choosing the minimum eigenvalue $\lambda$.

We then minimize $E(M_1, \ldots, M_\chi)$ using the same greedy random walk algorithm as above. At each step of the walk we decide which matrix $M_a$ to rotate at random. After each rotation one has to compute the new coefficient $g_a$ and properly update matrices $G, \Delta^{a,b}, F_0, F_{\text{imp}}$. This takes time $O(\chi n^3)$.
5.4. Numerical results. To benchmark the variational algorithm we chose the single impurity Anderson model [1]. This model has a Hamiltonian $H = H_0 + H_{\text{imp}}$, where

$$H_{\text{imp}} = U a_1^+ a_1 a_2^+ a_2 = \frac{U}{4} (-c_1 c_2 c_3 c_4 + i c_1 c_2 + i c_3 c_4 + I)$$

for some $U \geq 0$. This corresponds to the impurity of size $m = 4$ (we note that $m = 4$ is the smallest impurity size that gives rise to a non-trivial impurity model since any even Hamiltonian acting on $m \leq 3$ Majorana modes must be quadratic). For simplicity, we chose $H_0$ as the critical Majorana chain [26] with periodic boundary conditions:

$$H_0 = i \sum_{j=1}^{2n} c_j c_{j+1}, \quad c_{2n+1} \equiv c_1.$$ 

It is well-known [34,35] that $H_0$ has a unique ground state with parity $P = 1$ and the spectral gap proportional to $n^{-1}$.

Let $e_g$ be the ground energy of $H$. For each choice of $n$ and $U$ we numerically computed two numbers $e_g^+$ and $e_g^-$ such that

$$e_g^- \leq e_g \leq e_g^+.$$ 

The upper bound $e_g^+$ is the minimum energy found by the rank-$\chi$ variational algorithm. In our simulations we only used $\chi = 1$ and $\chi = 2$. The lower bound $e_g^-$ was computed using a version of the 2-RDM method commonly used in the quantum chemistry calculations [36]. Figure 2 shows the approximation error $e_g^+ - e_g^-$ as a function of the system size $n$ for several values of $U$. In all cases the rank-2 algorithm approximates the ground energy within an additive error less than $2 \times 10^{-6}$ and we were able to estimate $e_g$ within the first eight significant digits, see also Eq. (136).

| $n$  | $U = 1$          | $U = 8$          | $U = 64$         |
|------|------------------|------------------|------------------|
| 8    | -10.00932(5)     | -9.89010(8)      | -9.81220(9)      |
| 16   | -20.25487(5)     | -20.11633(4)     | -20.02426(8)     |
| 24   | -30.46084(8)     | -30.31627(5)     | -30.21953(6)     |
| 32   | -40.65683(1)     | -40.50931(8)     | -40.41024(6)     |
| 40   | -50.84854(5)     | -50.69954(7)     | -50.59907(2)     |

(136)
Acknowledgement. We acknowledge support from the IBM Research Frontiers Institute.

Appendix A: Proof of the Inner Product Formulas

In this appendix we prove the inner product formulas and the generalized Wick’s theorem of Sect. 2.4. Let $A$ be an arbitrary operator acting on the Fock space $\mathcal{H}_n$. Expanding $A$ in the basis of $4^n$ Majorana monomials $c(x)$, $x \in \{0, 1\}^{2n}$, one gets

$$A = \sum_x A_x c(x), \quad c(x) \equiv c_1^{x_1} \cdots c_{2^n}^{x_{2^n}}$$

for some coefficients $A_x$. Here and in the rest of this section all sums over binary strings have range $\{0, 1\}^{2n}$. An operator $A$ as above can be described by a generating function

$$A(\theta) = \sum_x A_x \theta(x), \quad \theta(x) \equiv \theta_1^{x_1} \cdots \theta_{2^n}^{x_{2^n}}.$$

where $\theta_1, \ldots, \theta_{2n}$ are formal variables obeying commutation rules of the Grassmann algebra, that is,

$$\theta_p^2 = 0, \quad \theta_p \theta_q = -\theta_q \theta_p.$$

An integral over Grassmann variables $\int D\theta$ is a linear functional defined by

$$\int D\theta \cdot \theta(x) = \begin{cases} 1 & \text{if } x = (1 \ldots 1) \equiv 1, \\ 0 & \text{otherwise} \end{cases}.$$

The action of $\int D\theta$ extends by linearity to an arbitrary function $A(\theta)$ by expanding $A(\theta)$ in the basis of Grassmann monomials $\theta(x)$. More details on the formalism of Grassmann variables can be found in [22,37]. Let $M$ be an anti-symmetric matrix of size $2n$. We shall consider $\theta = (\theta_1, \ldots, \theta_{2n})$ as a column vector and write $\theta^T$ for the corresponding row vector. Then

$$\theta^T M \theta \equiv \sum_{p,q=1}^{2n} M_{p,q} \theta_p \theta_q.$$

Suppose $\phi \in \mathcal{G}_n$ is a Gaussian state with a covariance matrix $M$ and let $A = |\phi\rangle \langle \phi|$. Wick’s theorem Eq. (21) can be rephrased as

$$A(\theta) = 2^{-n} \exp \left[ -\frac{i}{2} \theta^T M \theta \right]. \quad (137)$$

We shall need the following well-known formulas for Gaussian integrals:

$$\int D\theta \cdot \exp \left[ \frac{1}{2} \theta^T M \theta \right] = \text{Pf} (M), \quad (138)$$

$$\int D\eta \cdot \exp \left[ \theta^T \eta + \frac{1}{2} \eta^T M \eta \right] = \text{Pf} (M) \exp \left[ \frac{1}{2} \theta^T M^{-1} \theta \right]. \quad (139)$$

Here $\eta = (\eta_1, \ldots, \eta_{2n})$ is another vector of $2n$ Grassmann variables.
Now we can easily prove Eq. (22). Define a bilinear form

$$ \Gamma(x, y) = \sum_{1 \leq p < q \leq 2^n} x_p y_q \pmod{2}. $$

Here $x, y \in \{0, 1\}^{2n}$. Then $\text{Tr}[c(x)c(y)] = 2^n (-1)^{\Gamma(x,y)}$ if $x = y$ and $\text{Tr}[c(x)c(y)] = 0$ if $x \neq y$. Furthermore,

$$ \int D(\theta \eta) \cdot \theta(x) \eta(y) \exp(\theta^T \eta) = (-1)^n (-1)^{\Gamma(x,y)} $$

if $x = y$ and the integral is zero if $x \neq y$. Here both $\theta$ and $\eta$ are vectors of $2n$ Grassmann variables and $\int D(\theta \eta) \equiv \int D\theta \int D\eta$. Let $A, B$ be arbitrary operators on $\mathcal{H}_n$ and $A(\theta), B(\eta)$ be their generating functions. The above shows that

$$ \text{Tr}(AB) = (-2)^n \int D(\theta \eta) \cdot A(\theta) B(\eta) \exp(\theta^T \eta). \quad (140) $$

Suppose now that $A, B$ are projectors onto some pure Gaussian states $\phi_0, \phi_1$ with covariance matrices $M_0, M_1$ and parity $\sigma$. Substituting Eq. (137) into Eq. (140), taking the integral over $\eta$ using Eq. (139) and taking the integral over $\theta$ using Eq. (138) one gets

$$ \text{Tr}(AB) = 2^{-n} \text{Pf}(M_1) \text{Pf}(M_0 + M_1) = \sigma 2^{-n} \text{Pf}(M_0 + M_1). $$

Here we noted that $M_1^{-1} = -M_1$.

Next let us prove Eq. (23). Consider any even-weight strings $x, y, z \in \{0, 1\}^{2n}$ such that

$$ x + y + z = \mathbf{1}. \quad (141) $$

Here and below addition of binary strings is performed modulo two. Let $P \equiv (-i)^n c(\mathbf{1})$ be the total parity operator defined in Eq. (19). A simple algebra shows that

$$ \text{Tr}[Pc(x)c(y)c(z)] = i^n 2^n (-1)^{\Gamma(x,y)+\Gamma(y,z)+\Gamma(z,x)}. \quad (142) $$

Furthermore, the trace is zero whenever $x + y + z \neq \mathbf{1}$.

Suppose $\theta, \eta, \mu$ are vectors of $2n$ Grassmann variables. Let $D(\theta \eta \mu) \equiv D\theta D\eta D\mu$. A simple algebra shows that

$$ \int D(\theta \eta \mu) \cdot \theta(x) \eta(y) \mu(z) \exp[\theta^T \eta + \eta^T \mu + \mu^T \theta] = (-1)^n (-1)^{\Gamma(x,y)+\Gamma(y,z)+\Gamma(z,x)}. \quad (143) $$

Furthermore, the integral is zero whenever $x + y + z \neq \mathbf{1}$.

We shall say that an operator acting on $\mathcal{H}_n$ is even if its expansion in the basis of Majorana monomials includes only even-weight monomials. Let $A, B, C$ be any even operators on $\mathcal{H}_n$ and $A(\theta), B(\eta), C(\mu)$ be their generating functions. Comparing Eqs. (142, 143) one concludes that

$$ \text{Tr}(PABC) = (-i)^n 2^n \int D(\theta \eta \mu) \cdot A(\theta) B(\eta) C(\mu) \exp[\theta^T \eta + \eta^T \mu + \mu^T \theta] \quad (144) $$

Suppose now that $A, B, C$ are projectors onto some pure Gaussian states $\phi_0, \phi_1, \phi_2$ with covariance matrices $M_0, M_1, M_2$ respectively. Recall that any Gaussian state has a fixed parity, that is, $P\phi_\alpha = \sigma_\alpha \phi_\alpha$ for some $\sigma_\alpha = \pm 1$. Clearly $\text{Tr}(PABC) = 0$ unless all
states $\phi_0, \phi_1, \phi_2$ have the same parity: $\sigma_1 = \sigma_2 = \sigma_3 = \sigma$. Using Eqs. (137, 138) one gets

$$\text{Tr}(PABC) = \sigma \langle \phi_2 | \phi_0 \rangle \langle \phi_0 | \phi_1 \rangle \langle \phi_1 | \phi_2 \rangle = (-i)^n 4^{-n} \text{Pf} \left( \begin{bmatrix} -iM_0 & I & -I \\ -I & -iM_1 & I \\ I & -I & -iM_2 \end{bmatrix} \right).$$

This is equivalent to Eq. (23). To prove Eq. (24) let us come back to Eq. (144) and take a partial integral over $\mu$. Applying Eq. (139) and noting that $\text{Pf} (-iM_2) = (-i)^n \sigma$ one gets

$$\text{Tr}(PABC) = \sigma (-1)^n \int D(\eta) \cdot A(\eta) B(\eta) \exp \left[ \theta^T \eta - \frac{i}{2} (\eta - \theta)^T M_2 (\eta - \theta) \right].$$

Next let us take a partial integral over $\eta$. Applying Eq. (139) one gets

$$\text{Tr}(PABC) = \sigma i^n 2^{-n} \text{Pf} (M_1 + M_2) \int D\theta \cdot A(\theta) \exp \left[ -\frac{i}{2} \theta^T \Delta \theta \right],$$

where

$$\Delta = M_2 - (I - iM_2)^T (M_1 + M_2)^{-1} (I - iM_2).$$

Taking into account that $M_a^{-1} = -M_a$ one can rewrite $\Delta$ as

$$\Delta = (-2I + iM_1 - iM_2)(M_1 + M_2)^{-1}.$$

Finally, taking the integral over $\theta$ using Eq. (138) yields

$$\text{Tr}(PABC) = \sigma 4^{-n} \text{Pf} (M_1 + M_2) \text{Pf} (M_0 + \Delta).$$

This is equivalent to Eq. (24) since $PA = \sigma A$.

Next let us prove the generalized Wick’s theorem Eq. (26). Choose a Gaussian unitary $U$ such that $U c(x) U^\dagger = c_1 c_2 \cdots c_w$, where $w$ is the Hamming weight of $x$. Let $R \in O(2n)$ be the corresponding rotation defined by Eq. (16). Replacing each state $\phi_a$ by $U \phi_a$ is equivalent to replacing the covariance matrix $M_a$ by $R^T M_a R$. Thus suffices to prove Eq. (26) for the special case $c(x) = c_1 c_2 \cdots c_w$.

Define $C = c(x) \langle \phi_2 | \langle \phi_2 |$. We would like to compute the generating function $F(\mu)$ describing $C$. Using the standard Wick’s theorem Eq. (21) one gets

$$|\phi_2 \rangle \langle \phi_2 | = 2^{-n} \sum_y \text{Pf} (-iM_2[y]) c(y).$$

Here we noted that $\text{Tr}(c(y)^\dagger c(z)) = 2^n \delta_{y,z}$ and $c(y)^\dagger = (-1)^{\Gamma(y,y)} c(y)$. Therefore

$$C = c(x) \langle \phi_2 | \langle \phi_2 | = 2^{-n} \sum_y \text{Pf} (-iM_2[y]) (-1)^{\Gamma(y,x)} c(x + y).$$

It follows that $C$ has a generating function

$$C(\mu) = 2^{-n} \sum_y \text{Pf} (-iM_2[y]) (-1)^{\Gamma(y,x)} \mu(x + y).$$
Here $\mu = (\mu_1, \ldots, \mu_{2n})$ is a vector of $2n$ Grassmann variables. Let us construct a linear map $\Phi_x$ acting on Grassmann monomials such that

$$\Phi_x \cdot \mu(y) = (-1)^{\Gamma(y, x)} \mu(x + y)$$

for all $y \in \{0, 1\}^{2n}$. This would imply that

$$C(\mu) = \Phi_x \cdot 2^{-n} \exp \left[ -\frac{i}{2} \mu^T M_2 \mu \right].$$

It will be convenient to represent $\mu = (\mu', \mu'')$, where $\mu'$ has length $w$ and $\mu''$ has length $2n - w$. Then simple algebra shows that

$$(\Phi_x \cdot f)(\mu', \mu'') = \int D\tau \cdot \prod_{j=1}^w (1 + \tau_j \mu'_j) f(\tau, \mu'') = \int D\tau \cdot \exp \left[ \tau^T \mu' \right] f(\tau, \mu'').$$

(145)

Here $\tau = (\tau_1, \ldots, \tau_w)$ is a vector of $w$ Grassmann variables. Let $A(\theta)$ and $B(\eta)$ be the generating functions of projectors onto $\phi_0$ and $\phi_1$. Applying Eq. (144) and using the new definition of $C$ one arrives at

$$\text{Tr}(PABC) = \sigma \langle \phi_0|\phi_1\rangle \langle \phi_1|c(x)|\phi_2\rangle \langle \phi_2|\phi_0\rangle$$

(146)

and

$$\text{Tr}(PABC) = (-i)^n 2^n \int D(\theta \eta \mu) \cdot A(\theta) B(\eta) C(\mu) \exp \left[ \theta^T \eta + \eta^T \mu + \mu^T \theta \right].$$

(147)

Combining Eqs. (145, 147) one arrives at

$$\text{Tr}(PABC) = (-i)^n 4^{-n} \int D(\theta \eta \mu \tau)$$

$$\cdot \exp \left[ -\frac{i}{2} \theta^T M_0 \theta - \frac{i}{2} \eta^T M_1 \eta - i (\tau, \mu'')^T M_2 (\tau, \mu'')$$

$$+ \tau^T \mu' + \theta^T \eta + \eta^T \mu + \mu^T \theta \right].$$

Evaluating the integral using Eq. (138) gives

$$\text{Tr}(PABC) = (-i)^n 4^{-n} \text{Pf} \begin{pmatrix}
-i M_0 & I & -I \\
-I & -i M_1 & I \\
-I & -i D_x M_2 D_x & -J_x^T - i D_x M_2 J_x^T \\
J_x - i J_x M_2 D_x & -i J_x M_2 J_x^T \\
\end{pmatrix},$$

(148)

where $J_x$ is a matrix of size $w \times 2n$ such that $(J_x)_{i,j} = 1$ if $j$ is the position of the $i$-th nonzero of $x$ and $(J_x)_{i,j} = 0$ otherwise. Furthermore, $D_x$ is a diagonal matrix of size $2n$ such that $(D_x)_{j,j} = 1 - x_j$. Combining this and Eq. (146) proves the generalized Wick’s theorem Eq. (26).

To derive the simplified expression Eq. (27) it suffices to substitute $C = c(x)$ into Eq. (144) and evaluate the integrals using Eqs. (138, 139).
Appendix B: Containment in QCMA

We now consider the complexity of estimating the ground energy of a quantum impurity model to inverse polynomial precision. Formally, we consider the following decision problem (restated from Sect. 1.3).

Quantum impurity problem. We are given a quantum impurity model $H$ with $n$ fermi modes and impurity size $m = O(1)$, and two energy thresholds $a < b$ such that $b - a = 1/poly(n)$. We are promised that either $e_g \leq a$ (yes instance) or $e_g \geq b$ (no instance) and asked to decide which is the case.

In this section we prove the following theorem.

**Theorem 4.** The quantum impurity problem is contained in QCMA.

We first review some facts concerning the representation of fermionic states on a quantum computer. Quantum states of $n$ fermionic modes are represented using $n$ qubits in the following way: for each $x \in \{0, 1\}^n$, the Fock basis state $\prod_{i=1}^n (a_i^\dagger x_i)|0^n\rangle$ is identified with the $n$-qubit computational basis state $|x\rangle$. Majorana operators are represented via the Jordan–Wigner transformation:

\begin{align*}
c_1 &= X_1 \\
c_2 &= Y_1 \\
c_{2a-1} &= Z_1 \cdots Z_{a-1}X_a \\
c_{2a} &= Z_1 \cdots Z_{a-1}Y_a
\end{align*}

With this representation, a Gaussian state can be prepared efficiently on a quantum computer. A simple strategy to prepare any Gaussian state was given in Ref. [38]; we summarize it here for completeness.

Let a Gaussian state $|\Phi\rangle$ be specified up to a global phase by its covariance matrix $M$, as defined in Eq. (17). For each $i, j = 1, 2, \ldots, 2n$ and $\theta \in [0, \pi]$ define a unitary

$$U(\theta, i, j) = e^{i \frac{\theta}{2} c_i c_j}.$$ 

Using the Majorana commutation relations one can easily check that the state $\Phi'$ defined by

$$|\Phi'\rangle = U(\theta, i, j)|\Phi\rangle$$

has covariance matrix

$$M' = R(\theta, i, j)MR(\theta, i, j)^T$$

where $R(\theta, i, j)$ is a “Givens rotation” which acts nontrivially only on the subspace spanned by basis vectors $i, j$, and within this subspace its action is described by the $2 \times 2$ matrix

$$\begin{pmatrix}
\cos(\theta) & \sin(\theta) \\
-\sin(\theta) & \cos(\theta)
\end{pmatrix}.$$ 

Since $M$ is a $2n \times 2n$ real and antisymmetric matrix satisfying $M^2 = -I$, there is an $SO(2n)$ matrix $R$ such that $M = RM_R R^T$, where $M_R$ is the covariance matrix of a standard basis state, see Eq. (18). The matrix $R$ can be computed efficiently using linear
algebra, e.g., from the real Schur decomposition of $M$ [39]. It can then be decomposed as a product

$$R = R(\theta_q, i_q, j_q) \ldots R(\theta_2, i_2, j_2)R(\theta_1, i_1, j_1)$$

for some angles $\theta_1, \ldots, \theta_q$ and qubit indices $i_1, j_1, i_2, j_2, \ldots, i_q, j_q$, where $q = O(n^2)$. Such a decomposition can be computed, for example, using the strategy provided in Section 4.5.1 of the textbook Nielsen and Chuang [40] for decomposing a given unitary into two-level unitaries. We then have

$$|\Phi_1\rangle = e^{i\kappa}U(\theta_q, i_q, j_q) \ldots U(\theta_2, i_2, j_2)U(\theta_1, i_1, j_1)|y\rangle,$$

for some global phase $e^{i\kappa}$ and computational basis state $y \in \{0, 1\}^n$. From this expression it is evident that $|\Phi_1\rangle$ can be prepared efficiently, since the right hand side consists of $O(n^2)$ unitaries $U(\theta, i, j)$, each of which is an exponential of a Pauli operator. In the following we will only need to use the slightly weaker statement that there exists a polynomial sized quantum circuit which prepares $\Phi_1$ starting from $|0^n\rangle$.

We now give the proof of Theorem 4.

Proof. Let $H, a, b$ be given. Define $\gamma = (b - a)/4$ and consider the truncated Hamiltonian $H(\gamma)$ from Eq. (86). Here $H(\gamma) = H_0(\gamma) + H_{imp}$ where $H_0(\gamma)$ has spectral gap $\omega = \gamma/m$. The truncation lemma (Lemma 4) states that $|e(\gamma) - e_g| \leq \gamma$.

Therefore

$$e_g < a \implies e(\gamma) < a' \quad a' = a + (b - a)/4$$

$$e_g > b \implies e(\gamma) > b' \quad b' = b - (b - a)/4$$

(153)

Note $b' - a' = (b - a)/2 = 1/poly(n)$. Also note that $H(\gamma)$ can be computed efficiently given $H, b, a$; we need only diagonalize the free fermion Hamiltonian $H_0$ which takes time $O(n^3)$. We have shown that the solution to the quantum impurity problem for $H$ with precision parameters $a, b$ is equivalent to the quantum impurity problem for $H(\gamma)$ with precision parameters $b', a'$. Below we give a QCMA protocol for the latter.

We use Corollary 2 with $\delta = 0.01$ (say) and Hamiltonian $H(\gamma)$. Since $m = O(1)$, it implies that there exists a normalized state $\phi$ of the form

$$|\phi\rangle = \sum_{j=1}^{\chi} z_j |\theta_j\rangle \quad \chi = e^{O(\log(1/\gamma))} = poly(1/\gamma) = poly(n).$$

(154)

where $\{\theta_j\}$ are orthonormal Gaussian states, and where $\|\phi - \psi\| \leq 0.01$ for some ground state $\psi$ of $H(\gamma)$.

As discussed above, each Gaussian state $\theta_j$ can be prepared by a quantum circuit of polynomial size. This implies that there is also a polynomial sized quantum circuit which prepares $\phi$ with high probability (0.99, say) and a flag qubit indicating success. Indeed, the unitary

$$\sum_{j=1}^{\chi} |j\rangle\langle j| \otimes U_j$$

(155)
can be implemented with a circuit of size $O(\chi \log(\chi) \cdot \text{poly}(n))$, where the first register consists of $\alpha \equiv \lceil \log_2(\chi) \rceil$ ancilla qubits. To see this, note that Eq. (155) can be written as a product $\prod_{j=1}^{\chi} (X(j) \Lambda(U_j)X(j))$ where $X(j)$ is a product of Pauli $X$ operators such that

$$X(j)|1)^{\otimes \alpha} = |j)$$

and $\Lambda(U_j) = |1\rangle\langle 1|^{\otimes \alpha} \otimes U_j + (I - |1\rangle\langle 1|)^{\otimes \alpha} \otimes I$ is a multiply-controlled $U_j$ gate which can be implemented with standard techniques using $\alpha - 1$ additional ancilla qubits, one controlled-$U_j$ gate and $2\alpha - 2$ Toffoli gates (see Fig. 4.10 in [40]).

Applying Eq. (155) to the state $\chi^{(-1/2)} \sum_{i=1}^{\chi} |i\rangle|0^n\rangle$ one obtains $\chi^{(-1/2)} \sum_{i=1}^{\chi} |i\rangle|\theta_i\rangle$. We may then perform the projective measurement $\{|z\rangle\langle z| \otimes I, (I - |z\rangle\langle z|) \otimes I\}$, where

$$|z) = \sum_{j=1}^{n} z_j |j)$$

With probability $\chi^{-1}$ we obtain the desired state $\phi$. A quantum circuit which repeats this procedure $\Theta(\chi) = \text{poly}(n)$ times will produce $\phi$ with high probability.

Now we are ready to describe the QCMA protocol. The protocol begins with Merlin sending Arthur a classical description of a polynomial sized quantum circuit with an $n$-qubit output register and a flag qubit. Ideally, Arthur would like this to be the circuit which prepares $\phi$ with probability 0.99 (with the flag qubit indicating whether or not $\phi$ has been successfully prepared).

Arthur applies the given circuit to the all zeros input state and measures the flag qubit. If he obtains measurement outcome 1, then he performs the following test on the $n$-qubit output register, otherwise he rejects. Using phase estimation [40] on $e^{i\gamma H(\gamma)}$, he measures the eigenvalue of $H(\gamma)$ within precision $(b' - a')/4$. The parameters of the phase estimation are chosen so that the probability of failure is at most $\epsilon = 0.01$ (say). He accepts if the measured eigenvalue is at most $a' + (b' - a')/2$.

Let us now analyze the completeness and soundness of this protocol. In the yes case Merlin can send the circuit which prepares $\phi$ with probability 0.99. In this case there is a ground state $\psi$ with energy $e(\gamma) < a'$ such that $\|\phi - \psi\| \leq 0.01$, which implies $||\phi)\langle\psi||^2 \geq 1 - 0.01^2$. Thus, if the phase estimation succeeds, then with probability at least $1 - 0.01^2$ Arthur will measure an energy which is at most $a' + (b' - a')/4$ causing him to accept. Thus the total probability for Arthur to accept is the product of 0.99 (the probability that the flag qubit is measured to be 1), 0.99 (the probability phase estimation succeeds), and $1 - 0.01^2$ (the probability that Arthur accepts given that phase estimation succeeds). We have shown that in the yes case Merlin can provide a classical witness which causes Arthur to accept with probability at least 2/3.

Next consider the no case. In this case the ground energy of $H(\gamma)$ is at least $b'$. Thus any eigenvalue of $H(\gamma)$, when approximated within precision $(b' - a')/4$, is greater than Arthur’s threshold to accept, i.e., greater than $a' + (b' - a')/2$. This means that, regardless of the circuit provided by Merlin, the only way Arthur will accept is if the phase estimation fails (which occurs with probability at most 0.01). Thus, in the no case, Arthur rejects with probability at least 1/3.

Finally, note that Arthur’s computation has polynomial running time. He first performs the (polynomial-sized) circuit given to him by Merlin, and then performs phase estimation to precision $(b' - a')/4 = 1/\text{poly}(n)$ and constant error probability. This phase estimation requires Arthur to implement Schrödinger time evolution $e^{i\gamma H(\gamma)}$ for
times $t = \text{poly}(n)$. This can be done efficiently since $H(\gamma)$ is a sparse and efficiently row-computable Hamiltonian [41]. Indeed, since $H(\gamma)$ is a quantum impurity Hamiltonian it can be written as a sum of $n^2 + 2^n$ Majorana monomials, each of which corresponds to an $n$-qubit Pauli. \[\Box\]

References

1. Anderson, P.W.: Localized magnetic states in metals. Phys. Rev. 124, 41–53 (1961)
2. Kondo, J.: Resistance minimum in dilute magnetic alloys. Prog. Theor. Phys. 32(1), 37–49 (1964)
3. Wilson, K.G.: The renormalization group: critical phenomena and the Kondo problem. Rev. Mod. Phys. 47(4), 773 (1975)
4. Kouwenhoven, L., Glazman, L.: Revival of the Kondo effect. Phys. World 14(1), 33 (2001)
5. De Haas, W.J., Van Den Berg, G.J.: The electrical resistance of gold and silver at low temperatures. Physica 3(6), 440–449 (1936)
6. Georges, A.: Strongly correlated electron materials: dynamical mean field theory and electronic structure. AIP Conf. Proc. 715(1), 3–74 (2004)
7. Kotliar, G., Savrasov, S., Haule, K., Oudovenko, V., Parcollet, O., Marianetti, C.: Electronic structure calculations with dynamical mean-field theory. Rev. Mod. Phys. 78(3), 865 (2006)
8. Bauer, B., Wecker, D., Millis, A.J., Hastings, M.B., Troyer, M.: Hybrid quantum-classical approach to correlated materials. Phys. Rev. X 6, 031045 (2016)
9. Kreula, J.M., García-Álvarez, L., Lamata, L., Clark, S.R., Solano, E., Jaksch, D.: Few-qubit quantum-classical simulation of strongly correlated lattice fermions. EPJ Quantum Technol. 3, 11 (2016)
10. Gharibian, S., Huang, Y., Landau, Z., Shin, S.W.: Quantum Hamiltonian complexity. Found. Trends Theor. Comput. Sci. 10(3), 159–282 (2015)
11. Kitaev, A.Yu., Shen, A.H., Vyalyi, M.N.: Classical and Quantum Computation. American Mathematical Society, Boston (2002)
12. Schuch, N., Verstraete, F.: Computational complexity of interacting electrons and fundamental limitations of density functional theory. Nat. Phys. 5(10), 732–735 (2009)
13. Bini, D., Pan, V.Y.: Computing matrix eigenvalues and polynomial zeros where the output is real. SIAM J. Comput. 24(4), 1099–1115 (1998)
14. Wiegmann, P.B., Tsvelick, A.M.: Exact solution of the Anderson model: I. J. Phys. C: Solid State Phys. 16(12), 2281 (1983)
15. Kawakami, N., Okiji, A.: Exact expression of the ground-state energy for the symmetric Anderson model. Phys. Lett. A 86(9), 483–486 (1981)
16. Zolotarev, E.: Application of elliptic functions to questions of functions deviating least and most from zero. Zap. Imp. Akad. Nauk. St. Petersb. 30(5), 1–59 (1877)
17. Brod, D.J., Childs, A.M.: The computational power of matchgates and the XY interaction on arbitrary graphs. Quantum Inf. Comput. 14(11-12), 901–916 (2014)
18. Kraus, C., Cirac, J.I.: Generalized Hartree–Fock theory for interacting fermions in lattices: numerical methods. New J. Phys. 12(11), 113004 (2010)
19. Landau, Z., Vazirani, U., Vidick, T.: A polynomial time algorithm for the ground state of one-dimensional gapped local Hamiltonians. Nat. Phys. 11(7), 566–569 (2015)
20. Aharonov, D., Naveh, T.: Quantum NP—A Survey. arXiv:quant-ph/0210077, (2002)
21. Terhal, B.M., DiVincenzo, D.P.: Classical simulation of noninteracting-fermion quantum circuits. Phys. Rev. A 65(3), 032325 (2002)
22. Bravyi, S.: Lagrangian representation for fermionic linear optics. Quantum Inf. Comput. 5(3), 216–238 (2005)
23. Wimmer, M.: Efficient numerical computation of the Pfaffian for dense and banded skew-symmetric matrices. ACM Trans. Math. Softw. 38, 4 (2012)
24. Rubow, J., Wolff, U.: A factorization algorithm to compute Pfaffians. Comput. Phys. Commun. 182(12), 2530–2532 (2011)
25. Schliemann, J., Cirac, J.I., Kuš, M., Lewenstein, M., Loss, D.: Quantum correlations in two-fermion systems. Phys. Rev. A 64(2), 022303 (2001)
26. Kitaev, A.Yu.: Unpaired Majorana fermions in quantum wires. Physics-Uspekhi 44(10S), 131 (2001)
27. Löwdin, P.-O.: Quantum theory of many-particle systems I. Phys. Rev. 97(6), 1474 (1955)
28. Kennedy, A.: Approximation theory for matrices. Nucl. Phys. B Proc. Suppl. 128, 107–116 (2004)
29. Chiu, T.-W., Hsieh, T.-H., Huang, C.-H., Huang, T.-R.: Note on the Zolotarev optimal rational approximation for the overlap Dirac operator. Phys. Rev. D 66(11), 114502 (2002)
30. Gončar, A.A.: Zolotarev problems connected with rational functions. Sbornik: Mathematics 7(4), 623–635 (1969)
31. Nakatsukasa, Y., Freund, R.W.: Computing fundamental matrix decompositions accurately via the matrix sign function in two iterations: The power of Zolotarev’s functions. http://eprints.ma.man.ac.uk/2414/01/papersirevrevf_tosiam.pdf, (2015)

32. Anderson, G.D., Vamanamurthy, M.K., Vuorinen, M.: Functional inequalities for complete elliptic integrals and their ratios. SIAM J. Math. Anal. 21(2), 536–549 (1990)

33. Newman, D.J.: Rational approximation to $|x|$. Mich. Math. J. 11(1), 11–14 (1964)

34. Schultz, T.D., Mattis, D.C., Lieb, E.H.: Two-dimensional Ising model as a soluble problem of many fermions. Rev. Mod. Phys. 36(3), 856 (1964)

35. Pfeuty, P.: The one-dimensional Ising model with a transverse field. Ann. Phys. 57(1), 79–90 (1970)

36. Mazziotti, D.A.: Variational two-electron reduced density matrix theory for many-electron atoms and molecules: implementation of the spin-and symmetry-adapted T2 condition through first-order semidefinite programming. Phys. Rev. A 72(3), 032510 (2005)

37. Francesco, P., Mathieu, P., Sénéchal, D.: Conformal Field Theory. Springer, Berlin (2012)

38. Wecker, D., Hastings, M.B., Wiebe, N., Clark, B.K., Nayak, C., Troyer, M.: Solving strongly correlated electron models on a quantum computer. Phys. Rev. A 92(6), 062318 (2015)

39. Golub, G.H., Van Loan, C.F.: Matrix Computations. Johns Hopkins University Press, Baltimore (1996)

40. Nielsen, M.A., Chuang, I.L.: Quantum Computation and Quantum Information. Cambridge Series on Information and the Natural Sciences. Cambridge University Press, Cambridge (2000)

41. Aharonov, D., Ta-Shma, A.: Adiabatic quantum state generation and statistical zero knowledge. In: Proceedings of the Thirty-fifth Annual ACM Symposium on Theory of Computing, STOC ’03, pages 20–29, New York, NY, USA, ACM. (2003)

Communicated by M. M. Wolf