Computational Complexity of interacting electrons and fundamental limitations of Density Functional Theory

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One of the central problems in quantum mechanics is to determine the ground state properties of a system of electrons interacting via the Coulomb potential. Since its introduction by Hohenberg, Kohn, and Sham[1,2], Density Functional Theory (DFT) has become the most widely used and successful method for simulating systems of interacting electrons, making their original work one of the most cited in physics. In this letter, we show that the field of computational complexity imposes fundamental limitations on DFT, as an efficient description of the associated universal functional would allow to solve any problem in the class QMA (the quantum version of NP) and thus particularly any problem in NP in polynomial time. This follows from the fact that finding the ground state energy of the Hubbard model in an external magnetic field is a hard problem even for a quantum computer, while given the universal functional it can be computed efficiently using DFT. This provides a clear illustration how the field of quantum computing is useful even if quantum computers would never be built.

The difficulty of finding the ground state properties of a large system of interacting electrons originates both from the exponential dimension of the underlying Hilbert space and from the fermionic nature of the wave function. It is a problem encountered virtually everywhere in quantum chemistry as well as in condensed matter physics: for instance, the spatial configuration of a molecule is the one for which the energy of the interacting electrons moving in the nuclear potential, together with the electrostatic energy of the nuclei, becomes minimal. Similarly, a rich variety of phenomena in solid state physics, in particular conductance and magnetic phenomena, can be understood by considering electrons moving in the periodic lattice potential, including such exciting phenomena as high-temperature superconductivity and the fractional quantum Hall effect.

A system of N electrons is described by the Hamiltonian

$$H = \underbrace{-\tfrac{1}{2}\sum_{i=1}^{N}\Delta_i}_{=:T} + \underbrace{\sum_{1\le i<j\le N}\frac{\gamma}{|r_i-r_j|}}_{=:I} + \sum_i V(x_i) \qquad (1)$$

($\gamma > 0$, and $x_i = (r_i, s_i)$ with r_i position and s_i spin), where the potential V contains both an electrostatic field $\phi(r)$ and a magnetic field $\vec{B}(r)$ which couples to the spin (the coupling to the orbit can be neglected for our purposes, see Supplementary Material), and the problem is to find the ground state within the set of fermionic (i.e. antisymmetric) quantum states. Following the early work of Slater[3], Hohenberg, Kohn, and Sham[1,2] showed that this problem could be rephrased as a single-particle minimization problem, for the reason that the only problem-dependent part is the external potential V whose expectation value only depends on the local density, while the kinetic and interaction terms T and I are fixed and universal for all systems. Thus, the ground state energy is given by

$$E_0 = \min_{\rho}\left\{\mathrm{tr}(V\rho) + F[\rho]\right\} \ , \qquad (2)$$

where ρ is a single-electron density, and the functional F contains the problem-independent minimization over T and I,

$$F[\rho] = \min_{\Omega\to\rho}\mathrm{tr}\left[(T+I)\Omega\right] \ . \qquad (3)$$

Here, the minimization runs over all N-electron density operators Ω which give rise to the reduced density ρ. The central requirement for a good DFT algorithm is to find a suitable approximation to the universal functional, and indeed better and better techniques have been developed, making DFT the most widely used and most successful algorithm for treating interacting electrons.

However, as we show in this letter, there exist fundamental limits which constrain the ability to find a generally applicable and efficiently computable approximation to the universal functional, and thus put bounds on the applicability of DFT. To this end, we consider the 2D Hubbard model with local magnetic fields, which arises from the problem of interacting electrons for a specifically chosen lattice potential, and can thus be simulated using DFT. We first determine the computational complexity of solving the Hubbard model and show that it is among the hardest problems in the complexity class QMA, Quantum Merlin Arthur. QMA contains problems which are believed to be hard to solve even by quantum computers, but once a solution is found, it can be checked efficiently by a quantum computer. Thus, QMA encompasses the complexity class NP. We compare this to the difficulty of solving the Hubbard model using DFT with a suitable approximation of the functional at hand, and find that in that case the Hubbard model can be solved by a classical computer in a time polynomial in the number of electrons. This means that the existence of an efficient approximation to the functional would imply QMA=P, i.e. computing the functional to polynomial accuracy in the number of electrons is a QMA-hard problem, which poses fundamental limitations on the ability to approximate the functional in DFT. Of course, this does not mean that DFT is not applicable in practice: much lower (e.g. constant) accuracies will typically suffice, and DFT is indeed a highly successful method.

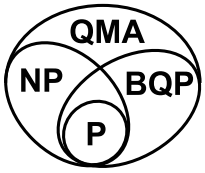

FIG. 1: The relevant complexity classes and their relations. While P and BQP are the classes of problems efficiently solvable by classical and quantum computers, respectively, NP (QMA) contains decision problems which are likely to be hard to solve by classical (quantum) computers, but where for positive instances, classical (quantum) proofs exist which can be checked efficiently by a classical (quantum) computer. All inclusions are believed to be strict. We show that solving the Hubbard model is among the hardest problems in QMA, while the existence of an efficient description of the universal functional in DFT would put it in P, leading to the collapse of all aforementioned complexity classes. This puts tight bounds on the existence of such functionals.

The 2D Hubbard model[4,5] describes a system of fermions hopping on a lattice. Although it typically appears as a phenomenological model for strongly bound electrons in solid state physics[6], it can be derived rigorously from (1) for an appropriate potential, as we show in the Supplementary Material. The Hubbard model with local magnetic fields is given by the Hamiltonian

$$H_{\text{Hubb}} = -t \sum_{<i,j>,s} a^\dagger_{i,s} a_{j,s} + U \sum_i n_{i,\uparrow} n_{i,\downarrow} - \sum_i \vec{\sigma}_i \cdot \vec{B}_i \ , \quad (4)$$

where $a^\dagger_{i,s}$ creates an electron of spin $s \in \{\uparrow,\downarrow\}$ on lattice site i, $<i,j>$ denotes nearest neighbors on the 2D square lattice, $n = a^\dagger a$, $\vec{\sigma}_i = (\sigma^{x,i}, \sigma^{y,i}, \sigma^{z,i})$, and $\sigma^{\alpha,i} = \sum_{s,s'} \sigma^\alpha_{ss'} a^\dagger_{i,s} a_{i,s'}$ with σ^α the Pauli matrices. The first term describes an electron tunneling from one site to the adjacent one without changing its spin, the second the on-site Coulomb repulsion between two electrons of different spin sitting on the same site, and the rightmost term contains the contribution from the magnetic field which imposes a local field at each site i – this is the only term which we can tune locally.

The 2D Hubbard model is of large interest on its own, as it is the minimal model that is believed to describe the physics arising in high-temperature superconductivity, quantum magnetism, and heavy fermions. Indeed, it is one of the most intensively studied models in solid state physics, making the investigation of its computational complexity interesting on its own. In the following, we show that computing its ground state energy up to polynomial accuracy is complete for the complexity class QMA, the quantum analogue of NP. A decision problem is in QMA if – although possibly hard to solve even by a quantum computer – every positive instance has a *quantum* proof which can be checked efficiently by a quantum computer. In particular, finding the ground state energy of a local spin system with an accuracy polynomial in the lattice size is in QMA: The ground state serves as a proof, as expectation values of local Hamiltonians can be estimated efficiently. Conversely, it has been shown that any circuit verifying a QMA proof can be encoded as a ground state problem[7,8], i.e., ground state problems are QMA-complete. (A problem is called complete for a class if it is among the hardest problems in this class, i.e., if any problem in the class can be reduced to it.) Using the same argument as before, finding the ground state energy of the Hubbard model is inside QMA, since it can be mapped to a spin system via the Jordan-Wigner transform: This allows to specify its ground state using spins, in such a way that it is possible to measure the ground state energy efficiently[9].

In the following, we show that the Hubbard model with magnetic fields is also a hard problem for QMA, and thus QMA-complete. To this end, we start from a class of Hamiltonians for which finding the ground state energy is known to be QMA-complete – i.e., as hard as finding the ground state energy of any local Hamilonian – and show that this problem can be reduced to finding the ground state energy of the Hubbard model with local magnetic fields. This is accomplished by a sequence of reductions, each of which reduces the previous Hamiltonian problem to a more restricted class of Hamiltonians. Each step makes use of perturbation theory constructions (so-called *gadgets*) such that the original Hamiltonian arises as the effective low-energy theory of the new Hamiltonian.

We start off with the Hamiltonian

$$H_{\text{Pauli}} = \sum_{<i,j>} \lambda_{ij} A_{(ij)} \otimes B_{(ij)} \quad (5)$$

defined on a 2D lattice with N spins, with $A_{(ij)}$ and $B_{(ij)}$ Pauli matrices and $|\lambda| \leq 1$, for which it has been proven that finding the ground state energy up to a polynomial accuracy $1/q(N)$ is QMA-hard[10]. Following Ref.[10], we call interactions of the form $\lambda_{ij} A_{(ij)} \otimes B_{(ij)}$ Pauli interactions.

We first show how the Pauli Hamiltonian (5) can be reduced to the 2D Heisenberg lattice with local fields (see Supplementary Material for details). To this end, we employ a chain of gadgets, all of which replace a two-qubit coupling by a chain of three qubits with a more restricted coupling. The idea is that by imposing a strong local field on the central ("mediator") qubit, the system will essentially be in the ground state of the central qubit – but there will be second-order processes in which an excitation hops from the left qubit to the central one and then to the right, or vice versa, yielding an effective coupling between the outer qubits. (The excitation can also hop back and give an extra local term, which however can easily be compensated by adjusting the local magnetic field.) Note that similar gadgets have already been used, e.g., in Refs.[10,15].

The full sequence of reductions to the Heisenberg lattice is illustrated in Fig. 2. In a first step, we reduce arbitrary Pauli couplings $\lambda A \otimes B$ to Pauli couplings with constant λ and $A \neq B$. We illustrate this with a $\lambda Y_l \otimes Z_r$ coupling (we use X for σ^x etc. in the following), which is obtained from three qubits with couplings $Y_l \otimes X_m \otimes \mathbb{1}_r + \mathbb{1}_l \otimes Y_m \otimes Z_r$ by putting a strong field in the XY plane on the central qubit: A short calculation shows that this indeed gives a $Y_l \otimes Z_r$ coupling, where the strength is given by the angle in the XY plane. The intuition behind is that e.g. a Y_l on the left qubit can excite the central qubit, and the excitation then hops to the

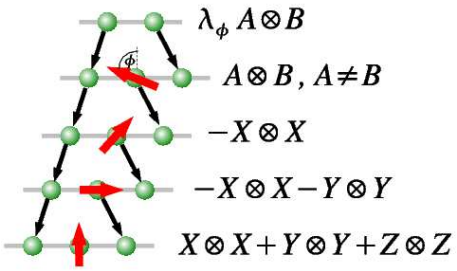

FIG. 2: Gadgets to reduce Pauli couplings to Heisenberg couplings. Each gadget works by inserting an extra spin in the middle which is subject to a strong local field, yielding the desired interaction in second order perturbation theory. A and B are Pauli matrices.

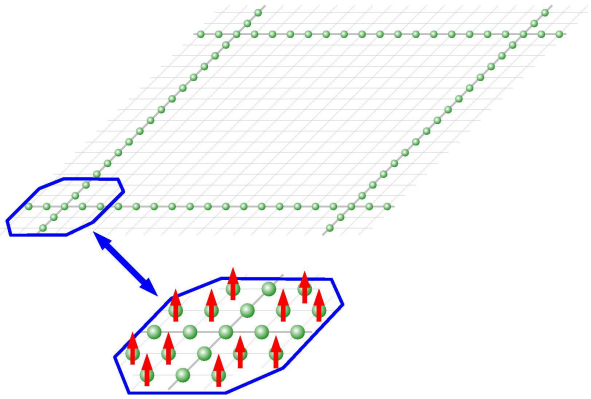

FIG. 3: The sparse Heisenberg lattice as obtained from H_{2D}, Eq. (5), using a sequence of gadgets. It can be reduced to a 2D Heisenberg lattice using the erasure gadget, where strong local fields are used to decouple unwanted qubits to leading order, as shown in the inset.

right qubit as a Z_r. In order for this hopping to be possible, the central field must not be along the X or Y axis, and correspondingly, the hopping amplitude is controlled by the overlap of the field with X and Y eigenvectors.

The second gadget reduces Pauli couplings $A\otimes B$ ($A\neq B$) to Ising couplings. This is achieved by essentially the same gadget as before: For $X_l\otimes Y_r$, take $X_l\otimes X_m\otimes \mathbb{1}_r + \mathbb{1}_l\otimes Y_m\otimes Y_r$ and place a strong field in $X+Y$ direction on the m qubit. In a next gadget, Ising couplings are reduced to two $X\otimes X+Y\otimes Y$ couplings: Placing a strong Y field on the central qubits only allows for the hopping of excitations via the $X\otimes X$ part of the coupling. Similarly, the above coupling is reduced to the Heisenberg interaction $X\otimes X+Y\otimes Y+Z\otimes Z$: A strong Z field prohibits hopping via the $Z\otimes Z$ term, whereas $X\otimes X+Y\otimes Y$ describes hopping in the $\{|01\rangle,|10\rangle\}$ subspace, which to second order yields the very same hopping term between the two outer qubits.

Putting these gadgets together, we have managed to reduce the QMA-complete Hamiltonian (5) to the Heisenberg Hamiltonian in a magnetic field on a sparse lattice. This can, in turn, be reduced to the full 2D Heisenberg lattice by using an "erasure gadget": putting strong fields on the qubits to be erased decouples them up to polynomial precision. We have thus shown that the 2D Heisenberg Hamiltonian in a magnetic field on a 2D square lattice,

$$H_{\rm Heis} = J\sum_{<i,j>}\vec{\sigma}_i\cdot\vec{\sigma}_j - \sum_i \vec{B}_i\cdot\vec{\sigma}_i\ , \qquad (6)$$

is QMA-complete, both for $J>0$ (which we use further on) and $J<0$. Note that the presence of a magnetic field is crucial for the construction, as it is the only set of parameters available to encode a computational problem.

The final step is to reduce the Heisenberg lattice to the Hubbard model (4). The procedure can be found, e.g., in Ref.[6], and has been included in the supplementary material: In (4), one chooses an on-site repulsion U very large as compared to t, and operates the system in the so-called half-occupancy regime where there are as many electrons as sites. (Note that this implies that a polynomial scaling in the lattice size equals a polynomial scaling in the number of electrons.) The tunneling is supressed as t/U, so that in the ground state each site will be occupied by exactly one electron, providing the desired spin degree of freedom. The coupling between the spins is achieved by a second-order process where one electron tunnels to an adjacent site, interacts with the other electron, and tunnels back. However, this can only take place if the spins form a singlet, giving rise to the effective Hamiltonian (6) up to a constant. As the process is of second order, we have that $J=t^2/U>0$, and the error from higher order processes is $O(N^3t^3/U^2)$; thus, U/t has to grow polynomially with the system size N.

All these gadgets can be combined straightforwardly: Firstly, the gadgets in one layer do not interact, as they never share a coupling term. It can thus be checked straightforwardly that to second order perturbation theory, there will be no cross-talk between the gadgets. Secondly, all gadget layers can be applied one after another, as long as the *total* strength of the previous gadgets is sufficiently smaller than the strong local fields of the new gadgets. Since the number of layers is constant, this can be achieved by choosing poly-scale field strengths, which allows for a polynomial scaling of the interaction strength as well as an arbitrary polynomial precision in energy. (See Supplementary Materials for details.)

Let us now turn our attention back to DFT and the problem of interacting electrons. As we show in the Supplementary Material, the Hubbard model (4) with arbitrary local fields arises from (1) for an appropriately chosen V. For this particular potential, one can explicitly write down the wave function $w_i(r)$ of each mode a_i to sufficient precision. Thus, the ground state wave function of the Hubbard model is supported by the $w_i(r)$, and consequently the single-electron density for the ground state of the Hubbard model must be of the form $\rho(r)=\sum\lambda_{i,s,s'}|w_i(r)|^2|s\rangle\langle s'|$. Since the functional (3) is convex and the physical $\lambda_{i,s,s'}$ form a convex set in $\mathbb{R}^{4N}$, the minimization (up to polynomial accuracy) can be carried out efficiently,[16] i.e., finding the ground state energy of the Hubbard model is in P. This implies that $\mathsf{P}^{\mathsf{UF}}=\mathsf{QMA}$ with UF an oracle for the universal functional, i.e. computing the functional is QMA-hard under Turing reductions.

Let us note that there are alternative ways to define $F[\rho]$, e.g. as the minimum over all *pure* N-electron states[11,12], in which case F is not convex. Yet, efficient computability (or even certifiablity) of F would still imply that one could give a certificate for the ground state energy, i.e. QMA would collapse to NP. This is considered very unlikely, thus implying that any reasonably defined F cannot be computed in NP.

Finally, DFT can also be based on a functional defined on two-electron densities, which can be computed efficiently[11,12]. In this case, the QMA-hardness of the problem arises from the fact that characterizing the set of allowed two-electron reduced states, the N-representability problem, is QMA-hard[9]; in fact, this provides an alternative proof of its hardness.

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APPENDIX: NP-completeness of Hartree-Fock

One of the precursors of DFT which is still widely used is the Hartree-Fock method. It is similar to DFT in that it reduces the N-electron equation to a problem of individual electrons moving in an external field which depends only on the average electron distribution. Different from DFT, Hartree-Fock is based on a particular ansatz for the wave function and is therefore not guaranteed to give the true ground state energy; on the other hand, it is an iterative method which can be applied without prior assumptions, whereas in DFT some *a priori* guess on the form of the universal functional has to be made.

The starting point is a Hamiltonian

$$\mathcal{H} = \sum H^{(1)}_{i,j} a^\dagger_i a_j + \sum H^{(2)}_{ij,kl} a^\dagger_i a^\dagger_j a_k a_l + \dots \ , \qquad (7)$$

which is local, meaning the series terminates at some fixed $H^{(r)}$, and with a number of fermionic modes $M \geq N$; if it is derived from two-particle interactions as in the Schrödinger equation (1), $r = 2$. The Hartree-Fock method approximates the ground state of this Hamiltonian using the ansatz $b^\dagger_N \cdots b^\dagger_1 |\Omega\rangle$ with $b_i = \sum u_{ij} a_j$ (where $|\Omega\rangle$ is the vacuum). Note that this corresponds to an antisymmetrized product of single-particle wave functions, which is how Hartree-Fock is usually presented.

In the following, we show that approximating the ground state energy using the Hartree-Fock method is an NP-complete problem. More precisely, we consider the problem of deciding whether the lowest energy of (7) within the Hartree-Fock ansatz is below some a or above some $b > a$. We show that the problem is inside NP for up to an exponential accuracy $b - a$ and for any r, and that for NP-completeness a polynomial accuracy $b - a < 1/\mathrm{poly}(N)$ and $r = 2$ are sufficient.

To see that the problem is in NP, note that a Hartree-Fock state is fully characterized by the u_{ij}'s, and that from there its energy can be computed efficiently. Conversely, the problem is shown to be NP-hard by mapping it to the ground state problem for Ising spin glasses which is known to be NP-hard: Given an $L \times L \times 2$ lattice of two-level spins $S_i = \pm 1$ with a nearest neighbor Ising coupling $\mathcal{H} = \sum J_{ij} S_i S_j$, $J_{ij} \in \{0, -1, 1\}$, determine whether the ground state energy is the minimum one allowed by the individual J_{ij}'s or not. Therefore, embed the $N = 2L^2$ classical spins into a fermionic system with $2N$ modes occupied by N fermions. The modes come in pairs (a_{2i}, a_{2i+1}), and a Hamiltonian term $\lambda n_{2i} n_{2i+1}$, $\lambda = O(N^2)$ penalizes double occupancy, so that in the ground state exactly one mode per pair is occupied, giving an effective spin degree of freedom[9]; the coupling $J_{ij} S_i S_j$ of these spins is realized as $J_{ij} \sum_{p,q=0,1} (-1)^{p+q} n_{2i+p} n_{2j+q}$. As the ground state of the system is a classical spin state, it can be expressed as a Hartree-Fock state where $b_i = a_{2i}$ or $b_i = a_{2i+1}$, respectively, and since the classical Hamiltonian has a constant gap while perturbations from the penalized subspace are at most $O(1/\lambda^2)$, a polynomial accuracy is sufficient to make the problem NP-hard.

SUPPLEMENTARY MATERIAL

1. Second order perturbation theory

We start with a Hamiltonian $H = H_0 \oplus H_1$ and a perturbation

$$V = \begin{pmatrix} V_0 & V_{01} \\ V_{10} & V_1 \end{pmatrix}$$

with $\|H_0\|, \|V\| \leq v$ and $H_1 \geq \Delta \gg v$, and want to show that the low-energy spectrum of $H_{\rm tot} = H + V$ is well approximated by $H_{\rm eff} = H_0 + V_0 - V_{01}H_1^{-1}V_{10}$. To this end, rotate $H_{\rm tot}$ by a unitary $U = e^S$,

$$S = \begin{pmatrix} 0 & X \\ -X^\dagger & 0 \end{pmatrix} ,$$

where $X = -V_{01}H_1^{-1} + V_{01}H_1^{-1}V_1H_1^{-1} - V_0V_{01}H_1^{-2} - H_0V_{01}H_1^{-2}$ is chosen such as to make the Hamiltonian as diagonal as possible. For systematic constructions of S for any order of perturbation theory, see Ref.[14]. By expanding S to second order in v/Δ, we obtain a new Hamiltonian

$$\tilde{H}_{\rm tot} = UH_{\rm tot}U^\dagger = \begin{pmatrix} H_{\rm eff} + O(\frac{v^3}{\Delta^2}) & O(\frac{v^3}{\Delta^2}) \\ O(\frac{v^3}{\Delta^2}) & H_1 + V_1 + O(\frac{v^2}{\Delta}) \end{pmatrix},$$

where all $O(\cdot)$ symbols are bounds in operator norm. Now compare this Hamiltonian with the block-diagonal Hamiltonian $\tilde{H}_{\rm diag}$ obtained from $\tilde{H}_{\rm tot}$ by setting the off-diagonal blocks to zero: The low-energy spectrum of $\tilde{H}_{\rm diag}$ is given by $H_{\rm eff} + O(\frac{v^3}{\Delta^2})$, and since $\|\tilde{H}_{\rm diag} - \tilde{H}_{\rm tot}\|_{\rm op} = O(\frac{v^3}{\Delta^2})$, it follows that all eigenvalues are $O(\frac{v^3}{\Delta^2})$ - close to each other, and thus the low-energy spectrum of $H + V$ is given by

$$H_{\rm eff} = H_0 + V_0 - V_{01}H_1^{-1}V_{10} + O(\tfrac{v^3}{\Delta^2}) \ . \qquad (8)$$

Note that when applying the gadgets to an N-qubit system with an extensive number of local perturbations, the error bound will depend on N since $v \propto N$.

2. Gadgets

Let us now turn towards the gadget constructions. Starting from (5), we want to show how its low-energy subsector can be obtained as an effective theory from (4). Let us first note that all perturbation gadgets of one level can be applied simultaneously, since they are second order gadgets and the transition term V_{10} is a sum of two-body terms which excite *one* qubit only; to return to the ground state subspace in the next step, this excitation has to hop to one of the adjacent sites. Thus, there will be no cross-gadget terms and the action of each layer of gadgets can be investigated on the level of a single gadget.

We aim to approximate (5) with strength $\lambda_{ij} \leq 1$ up to a precision $O(1/q)$, with $q \equiv q(N)$ a polynomial in N (we will in the following omit the parameter N for most polynomials). For A and B Pauli matrices, we can obtain a tunable Pauli coupling $\lambda_T A \otimes B$ from

$$V = \lambda_P A \otimes X \otimes \mathbb{1} + \lambda_P \mathbb{1} \otimes Y \otimes B \ , \qquad (9)$$

by acting with a Hamiltonian $H = B_P|e_\phi\rangle\langle e_\phi|$, $B_P \gg \lambda_P$, and the excited state $|e_\phi\rangle = |0\rangle - e^{i\phi}|1\rangle$. Then, to second order, the system is described by the effective Hamiltonian

$$H_T = +2\lambda_P^2/B_P \sin\phi\cos\phi \ A \otimes B + O(\lambda_P^3/B_P^2)$$

(up to a constant, and times the ground state projector on the middle qubit); note that when combining the gadgets, the total error grows with the third power of the total strength of V, and thus as N^3. As we aim to implement any $|\lambda_T| \leq 1$, we set $\lambda_P^2 = B_P$ and tune the actual value using ϕ. Choosing $\lambda_P = N^4 q$, $B_P = N^8 q^2$ [$N^4 q \equiv N^4 q(N)$], we find that the *total* error is at most $N^3 O(\lambda_P^3/B_P^2) = O(1/Nq)$ and thus much below the targeted precision $O(1/q)$. Note that in particular, this allows to split any Pauli interaction in two interactions of the form $X \otimes Y$, i.e. with two different Pauli matrices and positive sign.

Let us now show how such an $X \otimes Y$ coupling as in Eq. (9) can be reduced to Ising interactions. To this end, consider the Hamiltonian

$$V = -\lambda_I X \otimes X \otimes \mathbb{1} - \lambda_I \mathbb{1} \otimes Y \otimes Y + H_{\rm loc} \qquad (10)$$

and apply a field $H = B_I|e_{\pi/4}\rangle\langle e_{\pi/4}|$. Here, $H_{\rm loc}$ represents the local fields of the preceding gadget layers. They act on the qubits remaining after the present gadget, i.e. do not induce transitions to excited states, and are thus first-order terms which are left untouched in (8). We choose $B_I = N^{20}q^5 \gg N\lambda_I$, and $\lambda_I = N^{12}q^3 \gg \|H_{\rm loc}\| = B_P = N^9 q^2$, which results in an effective Hamiltonian

$$H_P = +\lambda_I^2/B_I X \otimes Y + O(\lambda_I^3/B_I^2) + H_{\rm loc} \ ,$$

for which $\lambda_I^2/B_I = \lambda_P$, and $N^3 O(\lambda_I^3/B_I^2) = 1/Nq \ll O(1/q)$. Note that due to rotational invariance, this construction holds for any type of Pauli coupling.

Ising interactions Eq. (10) can in turn be reduced to XX-type interactions,

$$V = -\lambda_{XX}(X\otimes X + Y\otimes Y)\otimes\mathbb{1} - \mathbb{1}\otimes(X\otimes X + Y\otimes Y) + H_{\rm loc} \qquad (11)$$

by putting a field in the Y direction, $H = B_{XX}(\mathbb{1} - Y)/2$. This cancels all Y contributions in the Hamiltonian, since $\langle 0_y|Y|1_y\rangle = 0$, and one remains with the X part of V,

$$H_{XX} = -2\lambda_{XX}^2/B_{XX} X \otimes X + H_{\rm loc} + O(\lambda_{XX}^3/B_{XX}^2) \ .$$

(The factor 2 is due to the fact that either an X on the left can excite the middle qubit, which then decays towards the right, or vice versa.) We choose $\lambda_{XX} = N^{28}q^7/4$ and $B = N^{44}q^{11}/8$, which ensures that $2\lambda_{XX}^2/B_{XX} = \lambda_I$, $B_{XX} \gg \lambda_{XX} \gg B_I$, and the total error is $1/Nq \ll O(1/q)$, as required.

In a last step, we reduce the Hamiltonian with XX type couplings to an antiferromagnetic Heisenberg

Hamiltonian with local fields. To this end, consider

$$V = \lambda_H \sum_{S=X,Y,Z} (S\otimes S\otimes \mathbb{1} + \mathbb{1}\otimes S\otimes S) + H_{\rm loc} - \dots \\ - \lambda_H^2/B_H (Z\otimes\mathbb{1}\otimes\mathbb{1} + \mathbb{1}\otimes\mathbb{1}\otimes Z) \quad (12)$$

and place a strong field in Z direction, $H = B_H(\mathbb{1} - \sigma_Z)/2$, on the central qubit. Intuitively, the $X\otimes X + Y\otimes Y$ part describes the hopping of an excitation from one side through the central qubit to the other side; since the excitation can also hop back to the original site, it however also induces an additional local field which is compensated by the extra term in Eq. (12). The effective Hamiltonian obtained is then

$$H_H = -2\lambda_H^2/B_H (X\otimes X + Y\otimes Y) \ ,$$

and by choosing $B_H = N^{92}q^{23}/512$, $\lambda_H = N^{60}q^{15}/64$, we find that $2\lambda_H^2/B_H = \lambda_{XX}$, $B_H \gg \lambda_H \gg B_{XX}$, and the total error is again $O(1/Nq)$.

By combining these gadgets, we find that each Pauli coupling can be reduced to a line of 16 Heisenberg couplings with variable local fields. Note that it should be possible to significantly reduce the order of magnitude of the fields by going to higher order perturbation theory: Each second order gadget couples the two outer qubits by an excitation hopping through the middle qubit. Therefore, it should be possible to choose all fields of equal magnitude and go to 16th order perturbation theory, which is the lowest non-vanishing order, and to which solely hopping terms contribute. Note further that one can decrease the length of the chain to 12 couplings (and thus to 12th order perturbation theory), as one can equally combine one XY Pauli and one Ising interaction to obtain an arbitrary Pauli coupling, including antiferromagnetic Ising couplings.

3. Erasure gadget

The sparse Heisenberg lattice Fig. 3a can be straightforwardly reduced to a full 2D Heisenberg lattice with local fields. To this end, add fields $H = B_e(1-\sigma_z)/2$ on all qubits to be erased, while

$$V = \lambda_H \sum_{<ij>} \vec{\sigma}_i \cdot \vec{\sigma}_j + \sum_i \vec{B}_i \cdot \vec{\sigma}_i$$

is the 2D Heisenberg lattice. Then, according to Eq. (8), $H_{\rm eff} = H_0 + V_0 + O(\|V\|^2/B_e)$, which yields the Heisenberg Hamiltonian on the sparse lattice. In particular, given that $\|V\| \le N\lambda_H$, by choosing $B_e = N^3\lambda_H^2 q$ we find that $B_e \gg V$, and the total error is $O(1/Nq)$.

4. Reduction from Heisenberg to Hubbard model

The final reduction step shows how the Heisenberg model can be reduced to the Hubbard model Eq. (2) (see, e.g., Ref. 6). To this end, choose an one-dimensional ordering of the Hubbard lattice, e.g. row-wise from left to right, and always place the spin-up mode before the spin-down mode. This results in a one-dimensional ordering of the modes of the Hubbard model, $(a_{1,\uparrow}, a_{1,\downarrow}, a_{2,\uparrow}, a_{2,\downarrow}, \dots)$. Now apply a Jordan-Wigner transform,

$$a_{i,s} \to \Big(\prod \sigma^z_{i',s'}\Big)\, \sigma^-_{i,s}$$

where the product runs over all (i',s') left of (i,s). This transforms (4) to a two-level system with a Hamiltonian $H+V$,

$$H = U\sum_i n_{i,\uparrow} n_{i,\downarrow} \\ V = -t \sum_{<i,j>,s} \sigma^+_{i,s}\big[\Pi\, \sigma^z_{k,s'}\big]\sigma^-_{j,s} \\ + \sum_j \Big[(B^x_j - iB^y_j)\sigma^+_{j,\uparrow}\sigma^-_{j,\downarrow} + \text{h.c.}\Big] + B_z(n_{j,\uparrow} - n_{j,\downarrow})$$

with $n = \sigma^+\sigma^- = |1\rangle\langle 1|$. We consider V as a perturbation to H, i.e. $U \gg t, \vec{B}$, and do a second-order expansion. Since we operate the system in the half-occupancy regime, the ground state of H satisfies $n_{i,\uparrow} + n_{i,\downarrow} = 1$, which makes the σ^z string in the tunneling term vanish on all but the sites i and j. The half-occupancy allows to interpret the ground-state subspace as a system of spin $\frac{1}{2}$ particles by grouping modes $(i,\uparrow)$ and $(i,\downarrow)$. The magnetic term in V contributes only to first order (and yields the magnetic field operator on the resulting two-level system), so that the second-order term is found by considering four sites $((l,\uparrow),(l,\downarrow),(r,\uparrow),(r,\downarrow))$, with a Hamiltonian $H+V$,

$$H = U(|11\rangle\langle 11|_l \otimes \mathbb{1}_r + \mathbb{1}_l \otimes |11\rangle\langle 11|_r) \ , \\ V = -t(\sigma^+\otimes\sigma^z\otimes\sigma^-\otimes\mathbb{1} + \mathbb{1}\otimes\sigma^+\otimes\sigma^z\otimes\sigma^- + \text{h.c.}) \ .$$

A straightforward calculation on the subspace $\{|1001\rangle, |0110\rangle\}$ – the only one with non-vanishing second order contributions – shows that this leads to a term

$$H = -\frac{4t^2}{U}(|01\rangle - |10\rangle)(\langle 01| - \langle 10|)$$

expressed in the effective spin $\frac{1}{2}$'s described above, which up to a constant equals the antiferromagnetic Heisenberg Hamiltonian $(2t^2/U)\vec{\sigma}\cdot\vec{\sigma}$. Choosing $U = N^8\lambda_H^3 q^2/8$ and $t = N^4\lambda_H^2 q/4$, we have that $U \gg t, \|B\| = O(NB_e)$, $2t^2/U = \lambda_H$, and the error $N^3t^3/U^2 \ll 1/Nq$ as desired.

Let us note that as with the gadgets before, no cross-terms appear when applying the gadgets together, as the only way to return to the ground state subspace in second order are processes within a single gadget.

5. Reduction of the Hubbard model to the Schrödinger equation

In the following, we show how finding the ground state energy of the Hubbard model with a local field up to $1/\text{poly}(N)$ precision can be reduced to answering the same question for the Schrödinger equation (where N is both the number of sites of the Hubbard model and the number of electrons).

Structure of the proof.—Let us first give an overview of the proof, highlighting the crucial steps. In the first part,

we use the kinetic term together with an appropriate external electrostatic potential in the Schrödinger equation [terms T and V in (1)] to construct an exactly solvable model with the following property: The Hamiltonian can be decomposed as

$$H = H_0 \oplus H_1 \ , \tag{13}$$

where

$$H_0 = -t \sum_{\langle i,j\rangle,s} a^\dagger_{i,s} a_{j,s} + O(N^{-2\tau+1}) + \text{const.} \tag{14}$$

and the constant is chosen such that $H_0 \leq -\Delta$, and with $H_1 \geq 0$. Note that beyond the gap above the H_0 band, we do not care about the properties of H_1.

In the second part of the proof, we show how to incorporate the magnetic field and the Coulomb interaction which will yield the on-site repulsion term. Loosely speaking, we will treat the Coulomb interaction as a perturbation to the original Hamiltonian, and obtain the on-site repulsion in first order perturbation theory. However, this cannot be done using the tools for perturbative expansions used for spin systems (cf. Sec. 1 of the Supplementary Material) due to the unbounded nature of the Coulomb interaction. Instead, we will use a direct estimate to bound the effect on the ground state energy which stems from off-diagonal elements of the Coulomb interaction (i.e. those coupling the H_0 and the H_1 subspace). We then find that the ground state energy of the Hubbard model with local magnetic fields equals the ground state energy of the Schrödinger equation with an appropriately chosen external potential up to $1/\text{poly}(N)$, as claimed. (Note that the result obtained by some perturbation expansions is stronger since the whole low-energy spectrum is reproduced; however, this is not necessary for the reduction.)

Before we start with the derivation, let us fix the desired scaling of the variables: We aim to obtain a Hubbard model (4) with arbitrary local fields on an $N := L_x \times L_y$ lattice, and with the following scaling of the parameters: $t = N^{-\tau}$, $B_{\max} = \max|B_i| = O(N^{-\tau})$, $U = \text{const.} \times N^{-\zeta}$, and a precision in energy of $O(N^{-2\zeta+2})$, where we have that $0 < \zeta < \tau - 3$. Note that the *relative* accuracy increases as ζ and τ are scaled up, which allows us to obtain the polynomial accuracies needed for the perturbation gadgets discussed above.

The exactly solvable hopping model.—We start by constructing the 2D hopping model. We first consider a 1D exactly solvable model, the Kronig-Penney model, from which we then construct an exactly solvable model in 3D. (We set up a 3D lattice since we consider the Schrödinger equation in three-dimensional space; the same reduction would also work in 2D right away.) The 1D Kronig-Penney model on $[0, L]$ with periodic boundary conditions is defined by

$$V(r) = -\mathcal{V} \sum_{n=0}^{L-1} \delta(r-n) \ , \tag{15}$$

where we choose $\mathcal{V} = \tau \log N$. This model is exactly solvable: The eigenfunctions are Bloch waves

$$\psi_k(r+n) = \tfrac{1}{\mathcal{N}} e^{ikn} \left[e^{-\kappa r} + Y e^{-\kappa(d-r)} \right] \tag{16}$$

(where $r \in [0,1]$, $n = 0, \ldots, L-1$), with

$$Y = \frac{e^{ik+\kappa} - 1}{e^{\kappa} - e^{ik}} = e^{ik} + O(e^{-\kappa})$$

and normalization $\mathcal{N}^2 = L/\mathcal{V} + O(e^{-\mathcal{V}})$.

The dispersion relation for the lowest Bloch band of the Kronig-Penney model can be approximately solved as

$$E_k = -\kappa^2 = -\mathcal{V}^2 - 4\mathcal{V} e^{-\mathcal{V}} \cos(k) + O(\mathcal{V}^2 e^{-2\mathcal{V}}) \ .$$

This band is the only one with bound states, with a gap of $\Delta = \mathcal{V}^2 - O(\mathcal{V} N^{-\tau})$ above. Expressing the Hamiltonian in the lowest Bloch band in terms of the creation/annihilation operators a_l corresponding to the Wannier functions $w_l = \sum e^{ikl} \psi_k / \sqrt{L}$, one finds

$$H_0^{\text{1D}} = -\mathcal{V}^2 \sum_l a_l^\dagger a_l - t \sum_{\langle i,j\rangle} a_i^\dagger a_j + O(L \mathcal{V}^2 N^{-2\tau}) \ , \tag{17}$$

where $t \equiv e^{-\mathcal{V}} = N^{-\tau}$.

In order to obtain a three-dimensional solvable model, we use a potential $V(r_1, r_2, r_3) = V(r_1) + V(r_2) + V(r_3)$ with the one-dimensional potentials of Eq. (15). This choice of the potential leads to a product ansatz for the wavefunction, where the behavior of the lowest band is still described by the hopping Hamiltonian (17), but on a three-dimensional lattice; the energy gap to the next band is still given by Δ, the gap of the 1D model. Using this potential, we can set up a $L_x \times L_y \times 1$ lattice, $N := L_x L_y$. Using (16), we find that the Wannier functions of the model are of the form

$$w_0(r) = \mathcal{V}^{3/2} e^{-\mathcal{V}|r|_1} + O(\sqrt{\mathcal{V}} e^{-\mathcal{V}}) \ , \tag{18}$$

and $w_i(r) = w_0(r-i)$, where $i = (i_1, i_2) \in \{0, \ldots, L_x - 1\} \times \{0, \ldots, L_y - 1\}$ is the site index in the 2D lattice. Thus, we obtain the system described by (14).

Clearly, we can include the spin degree of freedom without affecting the model at the current stage, as the Hamiltonian currently does not include any magnetic field. As a result, the Wannier functions get an an additional spin index, $w_{n,s}(r) \equiv w_n(r) \otimes |s\rangle$.

Treating magnetic field and Coulomb repulsion.—Let us now show how to account for the effect of the magnetic field and the Coulomb repulsion. We obtain the magnetic field of the Hubbard model by putting a magnetic potential

$$V_{\text{mag}}(r) = \sum \vec{B}_n \chi(r+n)$$

in (1). Here, $\chi(r) = (1 - \exp(-\mathcal{V}))^3$ for $-\frac{1}{2} \leq r_i \leq \frac{1}{2}$ and zero otherwise. This choice ensures the following:
i) $\langle w_{n,s}|V_{\text{mag}}(r)|w_{n,s'}\rangle = \langle s|\vec{B}_n \cdot \vec{\sigma}|s'\rangle$ yields the effect of the field B_n on the spin degree of freedom.
ii) $\langle w_{n,s}|V_{\text{mag}}(r)|w_{m,s}\rangle = O(\mathcal{V} N^{-2\tau+1})$ is sufficiently small for $n \neq m$, using (18); the unwanted contribution from the magnetic field is any state is thus $O(\mathcal{V} N^{-2\tau+3})$.
iii) For any state $|\chi\rangle$, $\langle\chi|V_{\text{mag}}|\chi\rangle \geq -N^2 B_{\max} = O(N^{-\tau+2})$. (This bound can e.g. be obtained by neglecting the antisymmetry of the wave function.)

Before incorporating the Coulomb term I, note that the strength γ of the Coulomb interaction can be tuned relative to the other terms by rescaling the spatial coordinates of the system; we choose $\gamma = N^{-\zeta}/2\mathcal{V}$. The Coulomb term I has properties very analogous to those of V_{mag}:
i) The on-site repulsion is $\langle w_{n,0} \otimes w_{n,1}|I|w_{n,0} \otimes w_{n,1}\rangle = 0.8984(\dots)N^{-\zeta} + O(\mathcal{V}^4 N^{-\tau-\zeta+2})$ [we explain the calculation of the integral, including the evaluation of the prefactor, later; the error term is from (18)]; again, by neglecting antisymmetry, this yields a bound $O(N^{-\zeta+2})$ for the total on-site repulsion in the lowest band.
ii) $\langle w_{n,s}\otimes w_{n',s'}|I|w_{m,t}\otimes w_{m',t'}\rangle = O(\mathcal{V}^4 N^{-\tau-\zeta+2})$ unless $n = n' = m = m'$, using (18); the unwanted cross-terms from the Coulomb repulsion are thus $O(\mathcal{V}^4 N^{-\tau-\zeta+4})$.
iii) For any state $|\chi\rangle$ (in particular for any state in the excited band), $\langle\chi|I|\chi\rangle \geq 0$.

Dealing with unbounded perturbations.—By using the properties i)-iii) above, we will now be able to show that the ground state energy of the total Hamiltonian $H_{\mathrm{tot}} = H_{\mathrm{ex}} + V_{\mathrm{mag}} + I$ is well approximated by the energy of $\Pi_0 H_{\mathrm{tot}} \Pi_0$, where Π_0 projects onto the lowest band of H_{ex} (which gives the first order perturbation expansion).

Let $|\psi\rangle \equiv \sqrt{1-p}|\phi\rangle + \sqrt{p}|\chi\rangle$ be a ground state of H_{tot}, where $|\phi\rangle$ is supported in Π_0 and $|\chi\rangle$ in the orthogonal subspace $\Pi_1 = 1 - \Pi_0$ of high-energy states. We claim that then, p is very small and thus $\langle\phi|H_{\mathrm{tot}}|\phi\rangle$ has almost the same ground state energy, i.e., the ground state energy of $\Pi_0 H_{\mathrm{tot}} \Pi_0$ is a good approximation to the ground state energy of H_{tot}. (Since we will find that p is very small, this actually also implies that the ground state of the projected Hamiltonian is close to the true ground state.)

The error made in the energy by replacing $|\psi\rangle$ by $|\phi\rangle$ is

$$\begin{aligned}\Delta E &= \langle\phi|H_{\mathrm{ex}} + V_{\mathrm{mag}} + I|\phi\rangle - \langle\psi|H_{\mathrm{ex}} + V_{\mathrm{mag}} + I|\psi\rangle \\ &= p\big[\langle\phi|H_{\mathrm{ex}} + V_{\mathrm{mag}} + I|\phi\rangle - \langle\chi|H_{\mathrm{ex}} + V_{\mathrm{mag}} + I|\chi\rangle\big] \\ &\quad + 2\sqrt{(1-p)p}\big[\mathrm{Re}\langle\phi|V_{\mathrm{mag}}|\chi\rangle + \mathrm{Re}\langle\phi|I|\chi\rangle\big]\end{aligned}$$

To bound ΔE, we use the following facts (obtained by combining the statements about V_{mag} and I made before):
i) $\langle\phi|H_{\mathrm{ex}} + V_{\mathrm{mag}} + I|\phi\rangle \leq -\Delta + O(N^{-\zeta+2})$;
ii) $\langle\chi|H_{\mathrm{ex}} + V_{\mathrm{mag}} + I|\chi\rangle \geq -O(N^{-\tau+2})$;
iii) From the Cauchy-Schwarz inequality,

$$\begin{aligned}\mathrm{Re}\langle\phi|M|\chi\rangle &\leq |\langle\phi|M|\chi\rangle| \\ &\leq \sqrt{\langle\phi|MM^\dagger|\phi\rangle\langle\chi|\chi\rangle} = \sqrt{\langle\phi|MM^\dagger|\phi\rangle}\end{aligned}$$

Combining i)-iii), this yields a bound

$$\Delta E \leq p(-\Delta + \alpha) + 2\sqrt{(1-p)p}\,\beta$$

with $\alpha = O(N^{-\zeta+2})$ [from i) and ii)], and $\beta^2 = \langle\phi|I^2 + V_{\mathrm{mag}}^2|\phi\rangle = O(N^{-2\zeta+2})$ (the dominating I^2 term can be derived solely from scaling arguments, see later). Using $\Delta \gg \alpha, \beta$, it is straighforward to show that the maximum of the above expression [found at $p = O(\beta^2/\Delta^2)$] is $O(\beta^2/\Delta) = O(N^{-2\zeta+2})$, which bounds the error in the ground state energy we make by replacing H_{tot} by $\Pi_0 H_{\mathrm{tot}} \Pi_0$.

Evaluation of Coulomb energies.—Let us now show how to compute the strength of the on-site repulsion from the Coulomb interaction. Following (18), we have to evaluate the integral

$$\mathcal{V}^6\gamma \int \mathrm{d}^3r\mathrm{d}^3s \frac{e^{-2\mathcal{V}(|r|_1+|s|_1)}}{|r-s|_2} = \frac{\mathcal{V}\gamma}{32} \underbrace{\int \mathrm{d}^3r\mathrm{d}^3s \frac{e^{-(|r|_1+|s|_1)}}{|r-s|_2}}_{c_U}$$

The latter integral is a constant, $c_U = 28.7496(\dots)$. Moreover, it is possible to compute c_U to any accuracy ϵ in a time $1/\mathrm{poly}(\epsilon)$ which is sufficient to obtain an efficient reduction. To this end, first rewrite the integral as

$$c_U = \int \mathrm{d}^3q \frac{1}{|q|_2} G(q)\ , \tag{19}$$

where $G(q)$ is the Greens function

$$\begin{aligned}G(q) &= \int \mathrm{d}^3r\mathrm{d}^3s\ e^{-(|r|_1+|s|_1)}\delta(r-s-q) \\ &= \prod_i (1+|q_i|)\, e^{-|q_i|}\end{aligned}$$

Rewriting (19) in spherical coordinates and integrating over r, we are left with

$$c_U = 8\int_0^{\pi/2}\mathrm{d}\phi \int_0^{\pi/2}\mathrm{d}\theta\ \frac{n(\phi,\theta)}{d(\phi,\theta)}$$

where $d(\phi,\theta) = ((\cos\theta + \sin\theta)\sin\phi + \cos\phi)^5 \geq 1$ and $n(\phi,\theta)$ are trigonometric polynomials. Since the integrand and its derivatives are bounded, the integral can be evaluated numerically to precision ϵ using a grid of size $1/\mathrm{poly}(\epsilon)$.

The effective Hamiltonian.—Putting all steps together, we obtain the Hubbard model (4) with tunneling $t = N^{-\tau}$, on-site repulsion $U = 0.8984(\dots)\,N^{-\zeta}$, and the desired magnetic fields. Collecting all error terms, one finds that the total error in the ground state energy is given by $O(N^{-2\zeta+2})$, as desired.

Remarks.—A few notes: First, the fact that we are using a δ-potential for our model does not affect our claims about DFT, since only the electron density, which is free of singularities, is passed to the functional; particularly, all these densities arise from N-electron states. Second, in the Schrödinger equation (1) we have omitted the coupling of the magnetic field to the orbit of the electrons: the variant of DFT arising from this approximation is known as "spin-density functional theory"[11,12], and our hardness result holds for exactly this variant. Note also that a coupling to the orbit would result in a so-called Peierls phase $e^{i\phi_{kl}}a_k^\dagger a_l$ in the tunneling term of the Hubbard model, which gives non-vanishing terms only for non-trivial loops, i.e. only from fourth order perturbation theory on, and can therefore be neglected.