



Interacting electrons, Density Functional Theory, and Quantum Merlin Arthur

Norbert Schuch¹ and Frank Verstraete²

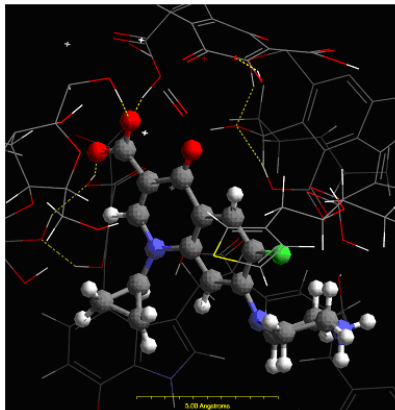
¹ Max-Planck-Institute for Quantum Optics, Garching, Germany

² University of Vienna, Vienna, Austria

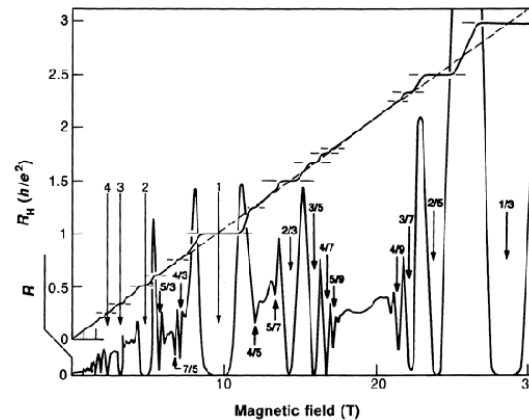
Introduction



- Understanding the behavior of **interacting electrons in an external potential** is a central problem in physics and chemistry



configuration
of molecules



The problem



Given Ham. for N electrons in an external potential $V(x)$,

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

contains magnetic term

compute its ground state energy $E_0 = \min_{\Omega} \text{tr}[\Omega H]$ (with Ω antisymmetric).

(in fact we always consider the decision problem INTERACTING ELECTRONS:

Decide whether $E_0(H) < a$ or $E_0(H) > b$, $b - a > 1/\text{poly}(N)$,

given that one of the two is the case.)

Is there any structure in H which allows to simplify the problem?

⊖ Depends on phases & correlations.

⊕ It is the same for any instance.

⊖ Depends on the instance.

⊕ Only depends on electron *density*.

Density Functional Theory



- Density Functional Theory (DFT): [Hohenberg, Kohn, Sham '64/'65]
Most widely used and successful method for simulating int. electrons.
- Here's the idea behind **Density Functional Theory**:

$$\begin{aligned} E_0[V] &= \min_{\Omega} \text{tr}[\Omega(T+I+V)] \\ &= \min_{\rho} \min_{\Omega \rightarrow \rho} \{ \text{tr}[\Omega(T+I)] + \text{tr}[\rho V] \} \\ &= \min_{\rho} \{ F[\rho] + \text{tr}[\rho V] \} \end{aligned}$$

... where $F[\rho] = \min_{\Omega \rightarrow \rho} \text{tr}[\Omega(T+I)]$ (the “**universal functional**”)
encapsulates the hard part of the optimization.

- Central task in DFT: Find **good approximations to universal functional**.
-

What do we show?



Efficiently computable and universally applicable approximation to the universal functional can not exist.

(based on complexity theoretic assumptions)

- Basic ingredients of the proof:
 - Solving INTERACTING ELECTRONS is **QMA**-hard.
 - Given $F[\rho]$, we can solve it efficiently.
 - ⇒ **Computing F is QMA-hard.**
- Actually, here's how it really works:
 - Solving the **Hubbard model** is **QMA**-complete.
 - The Hubbard model can be reduced to INTERACTING ELECTRONS.
 - Given $F[\rho]$ and using this reduction, the Hubbard model is in **P**.
- Furthermore ...
 - $F[\rho]$ can be defined differently but still places the Hubbard model in **NP**.
 - ⇒ **Those F reduce QMA to NP** (i.e. are hard to compute unless **QMA=NP**).

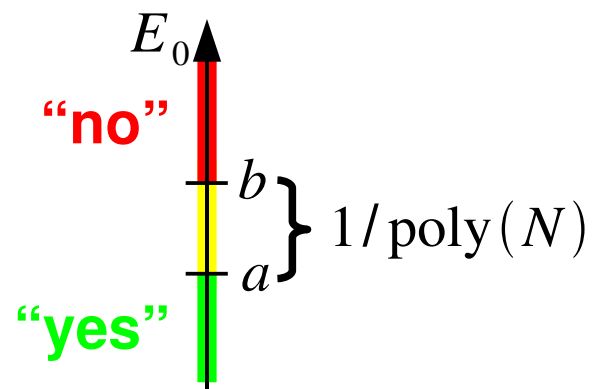
Quantum Merlin Arthur



- **QMA** (Quantum Merlin Arthur): quantum version of **NP** – the class of decision problems where “yes” instances have a quantum proof which can be verified by a quantum computer

- *ground state problems* are typical **QMA**-complete problems:

- Given a Hamiltonian H (from some class),
- and numbers a, b s.th. $b - a > 1/\text{poly}(N)$,
- with the promise that $E_0(H) < a$ or $E_0(H) > b$
- ... decide whether $E_0(H) < a$!



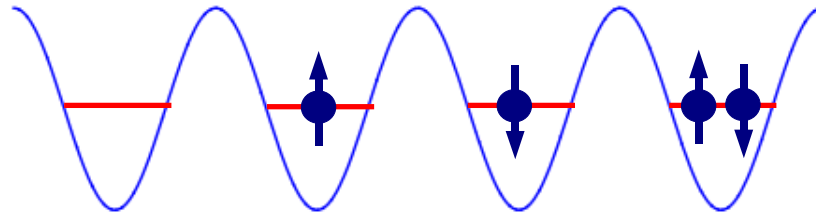
- More colloquially: Compute the ground state energy up to polynomial precision!

- In this talk: Solving X = computing the g.s. energy of X
= deciding the g.s. energy of X up to poly. accuracy

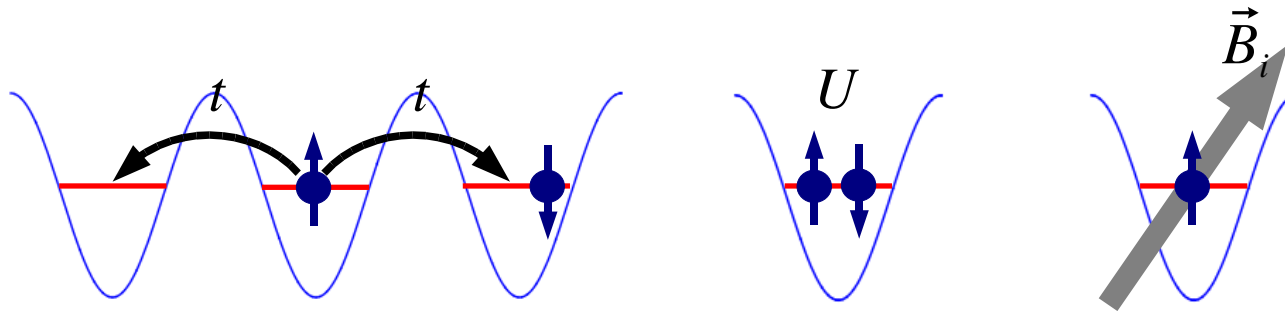
The Hubbard model



- The **Hubbard model** describes a system of fermions hopping on a lattice:



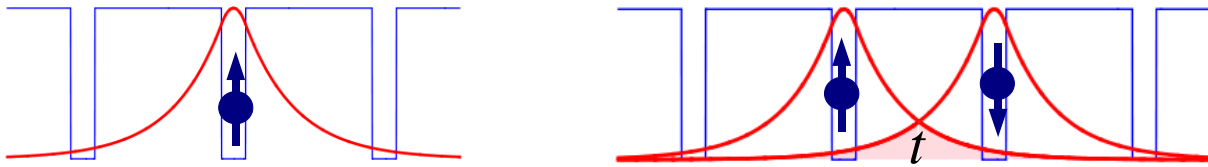
$$H_{\text{Hubb}} = -t \sum_{\langle i, j \rangle, s} a_{i,s}^\dagger a_{j,s} + U \sum_i n_{i,\uparrow} n_{i,\downarrow} - \sum_i \vec{B}_i \cdot \vec{\sigma}_i$$



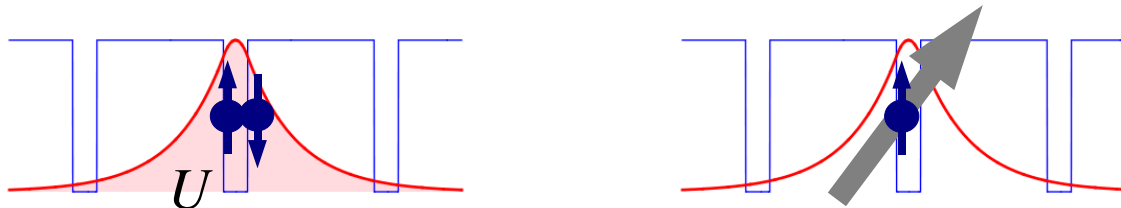
Reduction to INTERACTING ELECTRONS



- The Hubbard model can be reduced to INTERACTING ELECTRONS.
 - start from an exactly solvable lattice potential



- add the Coulomb interaction (and magn. fields) as a “perturbation”



⇒ Allows to simulate Hubbard model with same E_0 (up to $1/\text{poly}(n)$)

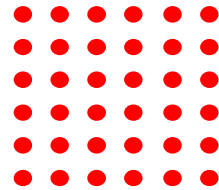
- Reduction also yields a set of basis states $\psi_i: \mathbb{R}^3 \rightarrow \mathbb{C}$ – corresponding to the modes a_i^\dagger – which support the optimal solution.

QMA-hardness of the Hubbard model



Any QMA
problem

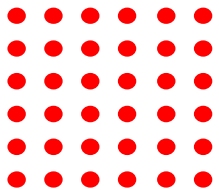
reduces to [Oliveira & Terhal '05]



2D lattice with Pauli couplings

$$H = \sum_{\langle i, j \rangle} \lambda_{ij} A_i \otimes B_j \quad (A, B \text{ Pauli mat.})$$

reduces to

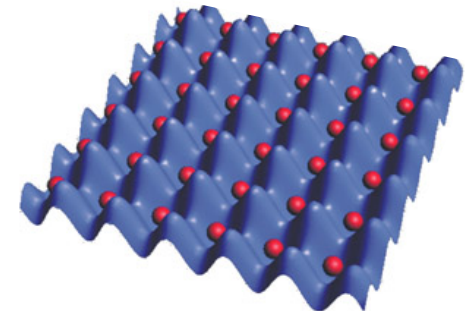


2D Heisenberg model w/ local fields

$$H_{\text{Heis}} = \frac{t^2}{U} \sum_{\langle i, j \rangle} \vec{\sigma}_i \cdot \vec{\sigma}_j - \sum_i \vec{B}_i \cdot \vec{\sigma}_i$$

reduces to

2D Hubbard model
w/ local fields

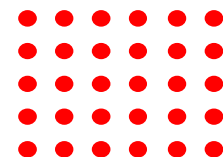


The reductions



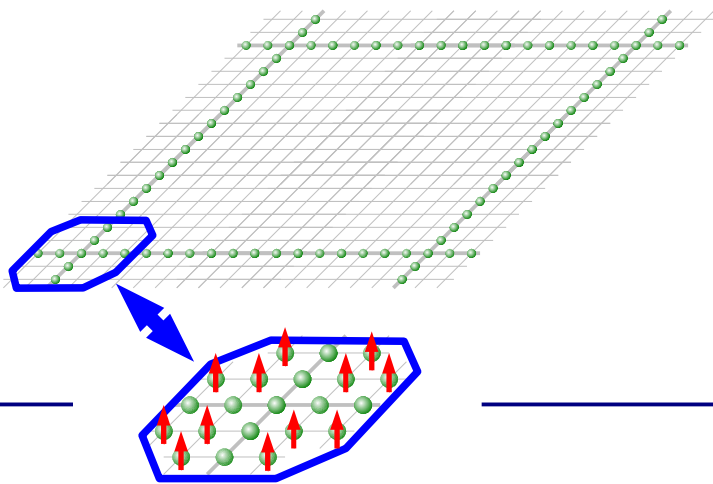
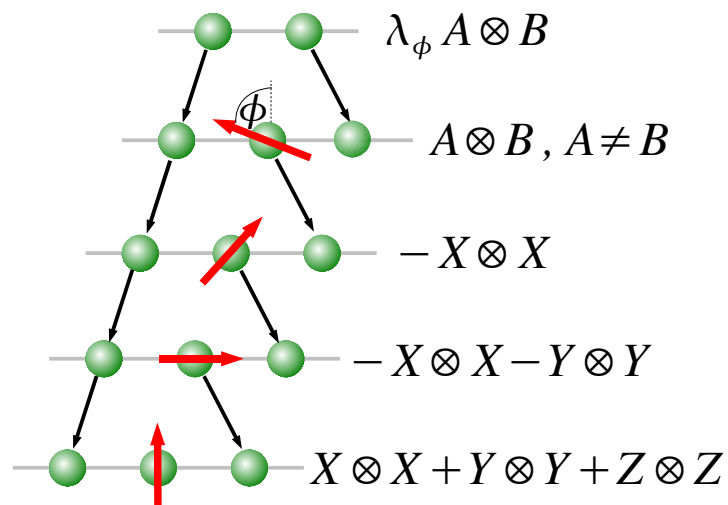
$$H = \sum_{\langle i, j \rangle} \lambda_{ij} A_i \otimes B_j \quad (A, B \text{ Pauli mat.})$$

$$H_{\text{Heis}} = \frac{t^2}{U} \sum_{\langle i, j \rangle} \vec{\sigma}_i \cdot \vec{\sigma}_j - \sum_i \vec{B}_i \cdot \vec{\sigma}_i$$

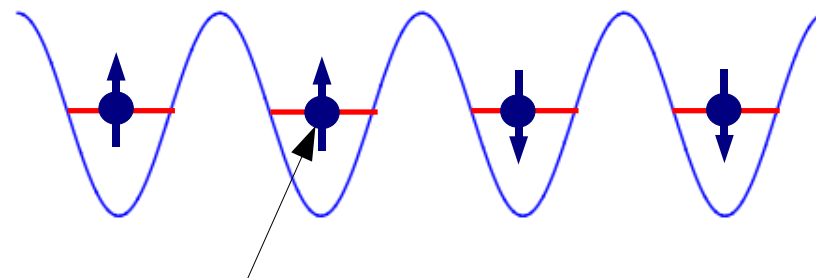


$$H_{\text{Hubb}} = -t \sum_{\langle i, j \rangle, s} a_{i,s}^\dagger a_{j,s} + U \sum_i n_{i,\uparrow} n_{i,\downarrow} - \sum_i \vec{B}_i \cdot \vec{\sigma}_i$$

- Perturbation gadgets:

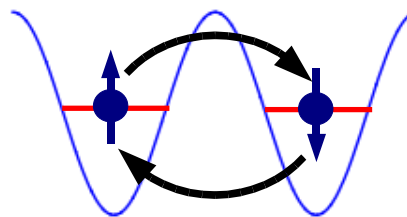


- Hubbard model at half-filling, $U \gg t$:



spin degree of freedom

- Interaction from 2nd order pert. theory:



only for singlets:

$$\vec{\sigma}_i \cdot \vec{\sigma}_j$$

Solving QMA problems with DFT



- Can an oracle for $F[\rho]$ help us to solve QMA problems?

i) Any QMA problem reduces to INT. ELECTRONS for some potential V .

ii) Basis $\psi_i(r)$ for g.s. known \Rightarrow ground state *electron density* is

$$\rho(r) = \sum_{\substack{i=1,\dots,N \\ s,s'=\uparrow,\downarrow}} w_{i,s,s'} |\psi_i(r)|^2 \otimes |s\rangle\langle s'|$$

& the $w_{i,s,s'}$ form a $4N$ -dimensional **convex set**.

iii) $F[\rho] = \min_{\Omega \rightarrow \rho} \text{tr}[\Omega(T+I)]$ is a **convex function**.

- Minimizing $E_0[V] = \min(F[\rho] + \text{tr}[\rho V])$ is a **convex optimization problem** – it is efficiently solvable (e.g. given an oracle deciding if $F[\rho] < a$ or $F[\rho] > b$).

\Rightarrow Approximating F efficiently is a QMA-hard problem!

Different functionals and QMA=NP



- Different ways to define the DFT functional. E.g.:

$$E_0[V] = \min_{|\psi\rangle} \langle \psi | T + I + V | \psi \rangle \quad \Rightarrow \quad F_p[\rho] = \min_{|\psi\rangle \rightarrow \rho} \langle \psi | T + I | \psi \rangle$$

Such functionals still satisfy $E_0[V] = \min \{ F_p[\rho] + \text{tr}[\rho V] \}$,
but **don't need to be convex** any more.

- However: Given an oracle for $F_p[\rho]$, it is still possible to eff. describe the ground state density, i.e. classically certify the ground state energy.
- $\Rightarrow F_p[\rho]$ cannot be computed efficiently unless **QMA=NP** (i.e. quantum proofs are no more powerful than classical ones – considered unlikely).

$$\mathbf{NP}^{F_p} = \mathbf{QMA}$$

(In fact $F_p[\rho]$ cannot even be computed in **NP** unless **QMA=NP**:
Otherwise, the optimal density ρ_0 + a certificate for the value of $F_p[\rho]$
serve as a certificate for the ground state energy).

DFT and N-representability



- DFT can also be done using **two**-electron densities ρ_2
- $F_2[\rho_2] = \text{tr}[(T + I)\rho_2]$ **can be computed efficiently!**
- However, $E_0[V] = \min_{\rho_2} (F_2[\rho_2] + \text{tr}[V\rho_2])$
requires to characterize the set of physical two-electron densities:

The N-representability problem!

- N-representability has been shown to be **QMA**-complete.
(Actually, this could also be used to prove it.) [Liu, Christandl, Verstraete '06]

Open questions



- **QMA**-hardness requires $1/\text{poly}(N)$ accuracy.
In practice however a constant accuracy will often suffice.
How hard is it to approximate $F[\rho]$ up to constant precision?
 - How hard is it to compute $F_p[\rho]$? Can we learn something about the relation of **NP** and **QMA** from there?
 - $F[\rho]$ can depend non-uniformly on the number N of electrons:
What can this tell us about non-uniform complexity classes?
 - DFT gives rise to a problem called *V-representability*:
 - Every potential V induces a ground state density ρ_0 .
 - *V-representability*: Given ρ , decide whether there is a V such that ρ is its ground state density.What is the computational complexity of V-representability?
-

Summary



- Solving INTERACTING ELECTRONS is **QMA**-hard
 - Solving the Hubbard model is **QMA**-complete
 - Using DFT, the Hubbard model can be solved efficiently
 - Approximating the universal functional is **QMA**-hard
 - Efficient computability of any admissible functional \Rightarrow **QMA=NP**.
- \Rightarrow Quantum complexity concepts pose fundamental bounds on the applicability of DFT.
-