

Schematic summary of the lectures
“Can we interface DFT and QIT?
And why is this relevant?”
‘DFT meets QIT’ ICTP-SAIFR International School,
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This is a schematic summary of the set of questions proposed and discussed during my lectures at the ‘DFT meets QIT’ ICTP-SAIFR International School. It also contains reference to the literature that – all or in part – has been discussed. This is just a sample of the literature available on the subject, and students are invited to look for more. [DFT: Density Functional Theory; QIT: Quantum Information Theory but also Quantum Information Technology].

OFTEN THE PROBLEM IS TO ASK THE RIGHT QUESTIONS...

1. DFT meeting QIT: why should we care?
2. Are there quantities of importance to QIT which could in principle be calculated using DFT?
3. Do we know how to express QIT quantities as functionals of the density?
4. If we don't know how to express a QIT quantity as functional of the density, what could we do?
5. Could we calculate only ground state properties?
6. Which are the limitations of the various methods?
7. Can we use QIT quantities to understand better DFT, or other 'many-body theories'?
8. Can we use 'DFT+QIT' concepts to understand quantum physics?
9. Are DFT and QIT communities speaking the same language?

1. DFT MEETING QIT: WHY SHOULD WE CARE?

- In its basic formulation, Density Functional Theory (DFT) ensures that, in principle, any ground state (GS) property of a (non-degenerate) quantum system can be written as a functional of the particle density.
- By using this property, it is, in principle, possible to avoid the complexity of the wave-function
- By the development of practical methods, mainly based on the solution of the Kohn-Sham (KS) equations, the various flavours of DFT have been successfully applied for various decades, and DFT has become by now one of the most reliable methods to calculate properties of (quantum) structures and materials.
- One key feature of DFT is that it allows for treatment of large quantum systems, while methods based on the wave function cannot (e.g. a problem is to store the coordinates of a many-body wave-function).
- Quantum Information Technologies, such as quantum computation, quantum simulations, etc, are based on quantum systems and, in principle, would like to address/use systems ever increasing in size, e.g. for increasing in size quantum computers and/or simulate larger and larger quantum systems and their interactions.
- Additionally, one important research line in quantum technologies is to design new nanostructures and/or materials which have the correct properties for the desired quantum device.
- Good reasons to interlace DFT and QIT could then be that DFT provides, in principle, a practical method to (i) calculate/simulate the properties of increasingly large interacting quantum systems and (ii) calculate and predict the quantum properties of (new) nanostructures and materials.
- In addition DFT and QIT are both based on the concept of quantum correlations, and so there is scope to look for links between the two fields, even if, as we will see, what is meant by 'quantum correlations' is different in the two fields.
- For its common usage DFT have been refined over the decades, but not towards QIT; which brings to the questions: within the state-of-the-art DFT, can we calculate quantities of importance to QIT using DFT? Which are the advantages/disadvantages? Which are the limits?

2. ARE THERE QUANTITIES OF IMPORTANCE TO QIT WHICH COULD IN PRINCIPLE BE CALCULATE USING DFT?

Desired quantities could be:

- excitations in quantum systems (e.g. for defining qubits);
- coupling strength between different degrees of freedom, e.g. between photons and excitons, phonons and electrons, to understand decoherence and/or how to drive the coupling between qubits;
- quantum dynamics, e.g. to simulate quantum gates in a quantum computer
- observables from specific quantum dynamics
- observables during a quantum dynamics
- quantum correlations such as entanglement and/or quantum discord
- quantum work,
- etc.

In principle excitations of quantum systems and observables during (or resulting-from) quantum dynamics could be calculated exactly using Time Dependent (TD) DFT; similarly GS properties (e.g. GS entanglement) could be calculated exactly using DFT.

In practice, apart from some cases, there are various problems related to (TD)DFT methods not been enough developed to calculate these properties.

There may be also more fundamental problems, a known one is that the calculation of the GS of complex many-body systems has been demonstrated to be a computationally hard problem.

Key issues are:

Do we know how to express QIT quantities as functionals of the density?

If so: how do the DFT approximations to the xc-potential behave?

If not, what could we do instead?

3. DO WE KNOW HOW TO EXPRESS QIT QUANTITIES AS FUNCTIONALS OF THE DENSITY?

THE CASE OF SITE-ENTANGLEMENT IN THE HUBBARD MODEL

Main reference: [1]

Other references cited in the discussion:

Parameterizations for the ground state energy E_{GS} [6] [7];

'Local' or 'single-site' entanglement[4];

'Local' or 'single-site' entanglement to identify quantum phase transitions[5];

Site entanglement in the homogeneous Hubbard Model[15];

Density functional for the local entanglement for the homogeneous Hubbard model[8];

Example of how 'quantum correlation' has a different meaning for different communities[8];

Non-homogeneous Hubbard model and the 'nested LDA' for the local entanglement[1];

Entanglement from experimental measurements of particle density: analytical density-functional for the site entanglement[9];

Caution about applying results from a model to a physical system [10, 11]

THE CASE OF THE CONCURRENCE FOR EXCHANGE-ONLY SPIN ENTANGLEMENT IN THE ELECTRON GAS

Main reference: [14]

See also lectures by Prof Giovanni Vignale within the same School.

4. IF WE DON'T KNOW HOW TO EXPRESS A QIT QUANTITY AS A FUNCTIONAL OF THE DENSITY, WHAT COULD WE DO?

Even when the explicit expression of the desired QIT quantity as functional of the density is unknown, there may be other approaches to exploit DFT for helping QIT.

For example:

- Can I find an ‘indicator’ for the QIT quantity of interest which is easy to calculate within DFT?
- Can I say ‘how good’ a DFT approximation would be for calculating a QIT quantity, even if I do not have the actual functional of the density?
- Can I use a functionals of the wave function plus ‘DFT tools’?

Find an ‘indicator’ for the QIT quantity of interest easy to calculate within DFT [2]

For concreteness let us focus on the entanglement, though the method can be extended to different QIT quantities.

We can think of an ‘entanglement indicator’ as a different quantity which follows a behaviour similar to the entanglement for all the parameter regimes of interest. So for example if the quantity grows we know the entanglement is growing, if it peaks so does the entanglement, etc. If we can identify a known functional of the density which behaves like this then:

- it is easy to calculate from DFT;
- we can have a lot of information about the entanglement;
- we can consider large systems;
- the numerical cost is relatively low.

In [2] Coe, Sudbery, and D’Amico analysed the particle-particle spatial entanglement for the Hooke’s atom, a system of 2 interacting electrons confined by a 3-dimensional parabolic potential of characteristic frequency ω . They found that a possible indicator of this type of entanglement is the ratio between the xc-energy to the total energy, $|E_{xc}/E|$.

The advantage of having an indicator based on the xc-energy, is that this is a key quantity within DFT and so many (approximate) ways, optimized over the decades, are available to calculate it.

However it must be noted that $|E_{xc}/E|$ is not always an entanglement indicator:

- It depends on the type of entanglement;
- It might depend on details of the system.

For example, $|E_{xc}/E|$ is not an entanglement indicator for the local entanglement in the Hubbard model.

I do not have the QIT quantity as functional of the density: can I still appraise a DFT approximation for calculating that QIT quantity? [2]

DFT methods are usually based on the xc-potential which is itself a functional of the density. However, in general, its functional form is not known, so, over the last 50 years, various approximations have been proposed which allow for accurate calculation of several physical properties for many different systems.

So let us assume that we do not have the actual functional of the density for the desired QIT quantity. However we know that, even if we had it, we would have to use one of the available approximations for the xc-potential to calculate it.

Could we appraise how good a specific approximation for the xc-potential would be, even if we do not have the desired quantity as functional of the density?

If we know the desired quantity as a functional of the wave-function, and if we are happy to perform this check on a relatively small system, the answer is, surprisingly, ‘Yes’.

This task can be achieved by considering the unique interacting system corresponding to a xc-approximation and its interacting wave-function.

Main reference: [2]

Other references cited in the discussion:

Results using evolutionary algorithms: [2]

Results using an accurate inversion scheme: [13]

Inversion scheme to find the external potential of the unique interacting system corresponding to a specific xc-approximation [12]

Could I calculate a QIT quantity using DFT tools, even if I do not know how to express the QIT quantity as functional of the density?

We can express our quantity of interest as a functional of the wave functions: can we use ‘somewhat’ the Kohn-Sham (KS) wavefunctions?

In certain cases we could indeed use a perturbation scheme based on the KS Hamiltonian.

Spatial particle-particle entanglement in Hooke’s atom and in quantum dots: [2] and , [13]

Calculation of quantum work: [3]

5. COULD WE CALCULATE ONLY GROUND STATE PROPERTIES?

Examples:

Quantum work: example of using KS quantities in function(al)s of wavefunctions and energies to calculate a property which is definitely not a GS property [3];

Excitations could be calculated from TDDFT;

Dynamics of observable could be calculated using TDDFT.

6. WHICH ARE THE LIMITATIONS OF THE VARIOUS METHODS?

Examples:

How close are the exact many-body and the KS wavefunctions? This is an open question.

KS wavefunctions could be used to estimate some types of entanglement but not all of them (see e.g. discussion in [2]).

Calculating the ground state as minimization of a functional is a problem demonstrated to be hard for a quantum computer.

7. CAN WE USE QIT QUANTITIES TO UNDERSTAND BETTER DFT, OR OTHER ‘MANY-BODY THEORIES’?

Examples:

Relationship between electron localization function and entanglement length[14]

Renormalization group methods and entanglement[16]

8. CAN WE USE ‘DFT+QIT’ CONCEPTS TO UNDERSTAND QUANTUM PHYSICS?

Examples:

Linking entanglement and quantum phase transitions via density functional theory[17]

Entanglement and DFT versus atomic shells and molecular bonds[14]

9. ARE DFT AND QIT COMMUNITIES SPEAKING THE SAME LANGUAGE?

Not yet:

- What do we mean by quantum correlations?
- Which quantum correlations are 'interesting' or 'useful' for each field?
- What do we mean by physical system? and by quantum state?

As we are not yet speaking the same language, it is useful to keep talking to each other.

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