Frustation and Dance Floors: Engineering Nanoconcepts with Quantum Mechanics

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May be you are a science-fiction movies fan and may be you have seen “I, robot” where Will Smith saved the Humanity using “nanites” which destroyed the main bad computer from inside. The nanites are an example of machines, of nanoids, of nanoscale robots we dream about in our century. They have a size of the order of few nanometers or in other words are 80000 times smaller than a diameter of human’s hair. Two centuries earlier, Jules Verne wrote about space, air, and underwater travel before navigable aircraft and practical submarines were invented, and before any means of space travel had been devised. Many of his predictions came to reality and others not. Thus it is justified to ask whether the nanites will be real or not and which of the today science-fictions ideas will survive?

Before transforming science-fiction into reality or to industrial applications, fundamental understanding of the interactions at the nanolevel is needed. This is one of the many goals of the IFF (FZ-Jülich) which lead to the two novel concepts presented in this manuscript: nanodominos and nanosonars. These are the results of computer simulations [1, 2, 3] which show how the intrinsic properties of electrons, such as being a little magnet and the way it propagates in a material, can be used to engineer nanodevices for storing data, for transmitting information from one point to another, for scanning surfaces and for drawing maps of underlying buried objects. A nanite will need all these options in order to swim for example in bloodstreams, cleaning arteries while shooting cancer cells of human beings. Indeed, it would need to perform logical operations and to see around. Nanodominos and nanosonars are very attractive concepts not only because of their easy applicability by the actual available experimental methods but for the concept of nanites .

Nanodomino:

Storing increasing amounts of data on increasingly smaller spaces and performing logical operations using increasing smaller amount of energy are two of the prerequisites for further progress in information technology. This requires the investigation of the magnetic behavior at the atomic-scale. Due to the electron's intrinsic property of carrying a minimagnet, they create a magnetic moment in atoms where they work together as a collective entity. Surprisingly, when looking at the magnetic moments in rows of individual manganese atoms on a nickel surface, socalled nanowires, we in Jülich discovered a kind of domino effect. We noticed that the magnetic configuration of these nanowires differed depending on their length; and one atom matters! Astonishingly, only one atom more or one less makes a drastic difference. When the number of atoms is odd, the orientation of neighboring magnetic moments are antiparallel, and when the number is even, they line up in a toppled compromise position between parallel and antiparallel. Adding an atom at the end of the nanowire or taking one away simultaneously changes the magnetic configuration of the entire wire. Just like a row of dominos, the magnetic moments topple over. However, this is where the analogy ends because the effect can be completely reversed in contrast to dominos that have toppled over. This behavior is a pure nano-effect which cannot be observed for bulk materials.

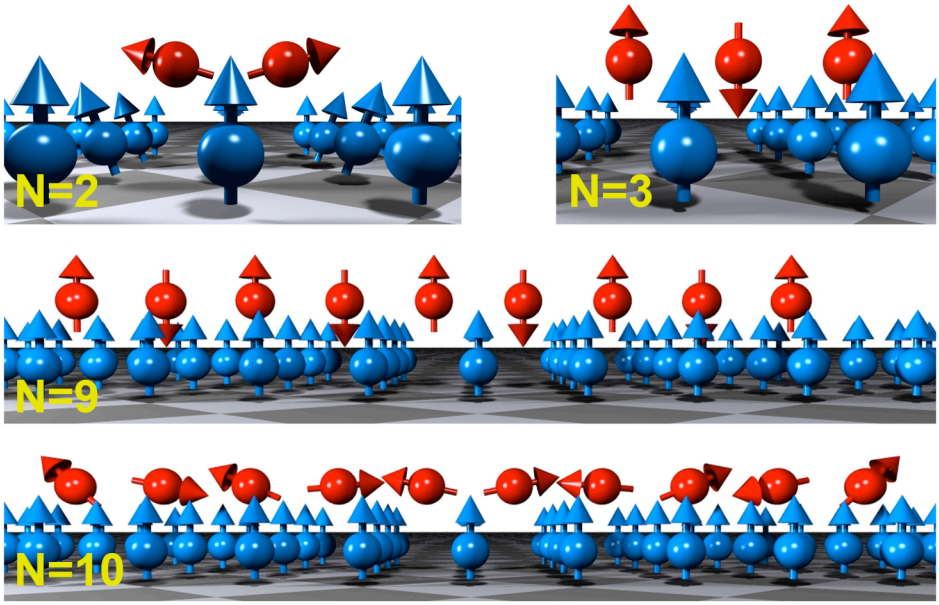

Figure 1: The magnetic moments of a row of manganese atoms (red) organize themselves in an antiparallel fashion on a nickel surface (blue) when their number N is odd, e.g. 3 or 9. When their number is even, say 2 or 10, the magnetic moments take up a compromise position.

What is the physics behind these nanodominos? Assume there are two atoms of iron separated by a quarter of a nanometer. They like to have their magnetic moments pointing in the same direction and parallel to each other. This is called ferromagnetic coupling. On the other hand, two atoms of manganese like to have their moments parallel to each other but pointing in opposite directions. This is called antiferromagnetic coupling. These different preferred couplings are designed by the number of electrons in each atom. What happens when an additional manganese atom is brought at an equidistant position from the two previous atoms (Figure 2)? The magnetic moment of this third atom does not know what to do! Either it couples antiferromagnetically to one manganese atom and makes the other one unhappy or switches its magnetic orientation to make the second manganese atom happy which the first atom would not appreciate. This situation called magnetic frustration is very often seen in nature. What happens at the end is that the magnetic moments rotate such that a compromise is found. In this case a rotation angle of 120 degrees between the magnetic moments removes the frustration.

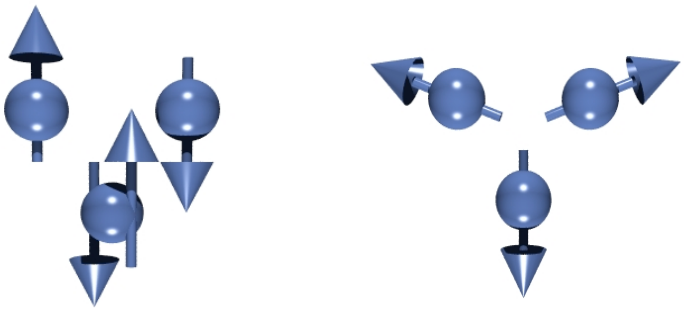

Figure 2: Example of magnetic frustration seen with antiferromagnetic manganese atoms. Frustration is obtained when all three atoms want to couple antiferromagnetically (left) leading to a non-collinear magnetic state (right).

Imagine that the third manganese atom is replaced by a ferromagnetic surface of nickel. The simulations show that one single manganese atom like very much to couple in a parallel fashion to the nickel atoms. Thus, frustration occurs since both manganese atoms want also to couple antiferromagntically to each other. The compromise is found with the manganese moments aligned antiparallel to each other and roughly perpendicular to the substrate moments (Figure 1 for N=2). An additional magnetic interaction brought by a possible third manganese atom sitting very close to the previous couple destroys the frustration and stabilizes the pure anti-parallel behavior. This leads to the even-odd effect for the longer wires. Wires with even number of atoms are frustrated and thus have a compromised magnetic configuration while odd wires are non-frustrated with an anti-parallel magnetic behavior. At the end, we witness a very nonlocal phenomena. Something is changed at the end of a long wire and the property across the entire chain changes.

This magnetic effect makes magnetic switches and logic elements conceivable on an atomic scale. Since the information on a hard disk is stored in terms of the binaries 0 and 1, the toppled dominos can represent the bit 0 while the untoppled ones would be the bit 1. Thus, the dominos cascades can be used for transport of a single bit of information from one location to another. They can be set in patterns that perform logical operations. Such a device would be important for the artificial brains of the nanites.

After having seen how the electron's minimagnet can be used for engineering a nanodomino, the next section is devoted to the paths followed by the electron when traveling in a material and their possible application in a nanosonar concept.

Nanosonar:

What happens if a stone is thrown in a lake? The additional volume creates waves or ripples on the surface (Figure 3 - left). The same effect happens when a foreign atom is buried below a surface. The sea of electrons, initially present in the material, reacts and tries to screen the additional foreign electrons leading to oscillations (Figure 3 - right).

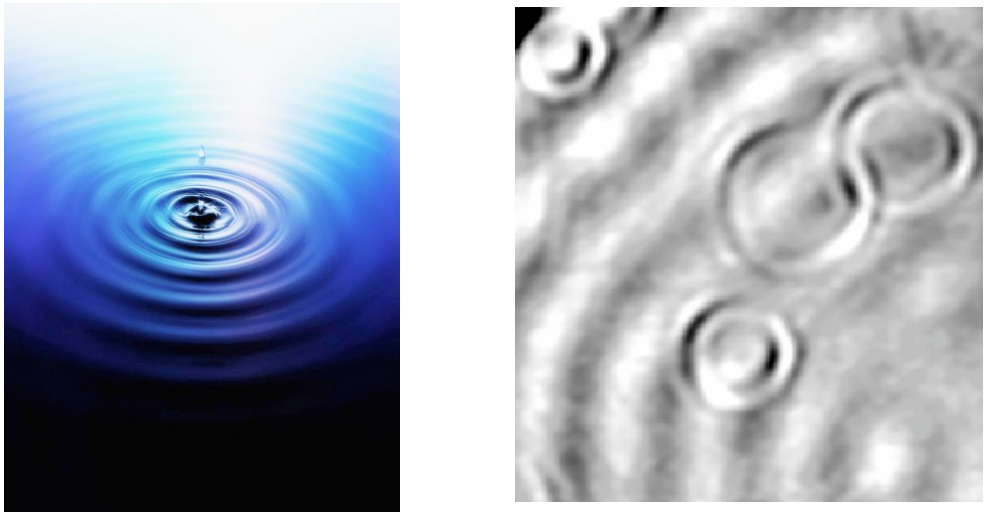

Figure 3: Ripples on water surface produced by an external object (left) and ripples on sea of electrons due to foreign atoms buried below copper surface (right)[4].

These oscillations can be used in a nanosonar device which would allow for example the detection of buried objects below surfaces and the investigation of their electronic and magnetic properties. What is sonar in our macro-life? **Sonar** (for **SO**und **NA**vigation and **R**anging) is a technique that uses sound propagation (usually underwater) to navigate, communicate, to detect other vessels or to scan deep underwaters. The principle is that a sound wave is emitted which propagates till it hits an object or a surface and is reflected back (Figure 4). Knowing the time needed for the reflection and the speed of sound we can determine the distance to the underwater object.

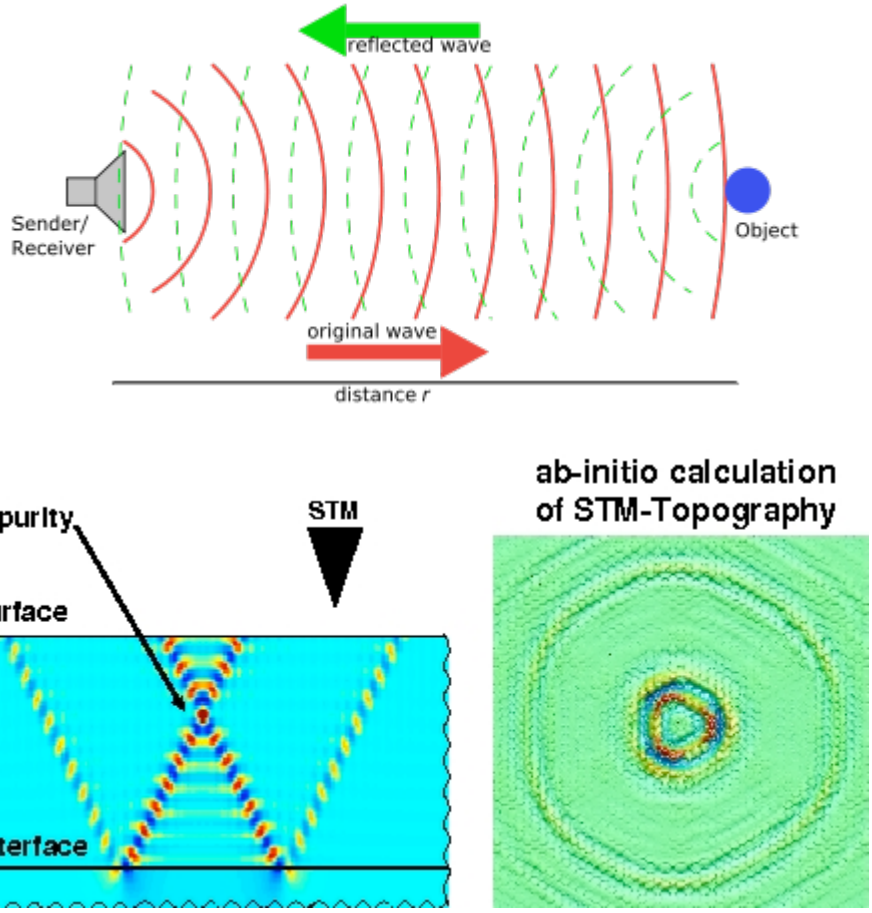

Figure 4: Upper figure: Concept of a sonar where emitted waves are reflected back at a given object; lower figures: a nanosonar is very similar with electron waves propagating instead of sound. Reflection at a buried impurity leads to a first ring while reflection at an interface leads to a second wider ring. The colored green picture corresponds to a surface with a size of 100nm x 100nm obtained with our simulations.

This concept is exactly applicable at the nanolevel where the main tool is the scanning tunneling microscope (STM) allowing the measurements of electron distributions on surfaces. With the nanosonar, the sound waves are replaced by the electron waves. Whenever the electrons hit a foreign object, they are reflected and seen on the surface by STM. This, in fact, would be the only possible analogy to the macrosonar we know. Indeed when the electrons are in motion in a solid they do not follow fortuitous paths. They follow well-assigned roads, roads created by the subatomic environment. These roads can be as big as highways with speeds as on the Autobahn, or can look like small village low-speed streets with a barrage at the end. This makes the electrons appear in some places or directions and disappear in

others just like ghosts.

If the roads were the same in all directions, the electron ripples observed on the surface would be cylindrical as the ones you would see if you throw a stone in a lake. The left pictures in Figure 5 show two examples of electron oscillations observed on two surfaces: copper along two particular orientations, one called (111) and one along the (100) orientation. On both surfaces the oscillations are localized but in one case their shape resembles a triangle and in the other case their shape is more like a square. Clearly, the paths followed by the electrons are not the same in all directions. How are these roads designed? The answer is a very important physical property of materials called Fermi surface. In condensed matter physics, this is an abstract concept useful for predicting the thermal, electrical, magnetic, and optical properties of metals, semimetals, and doped semiconductors. In fact, a solid is like a desk with many drawers. Every electron can occupy only one energy state, which is like a drawer in which is exactly one electron, starting from the lowest energy. The last drawer corresponding to the highest occupied energy defines the Fermi surface. The shape of this surface is derived from the periodicity and symmetry of the crystalline lattice. When the Fermi surface is a sphere, the roads are all alike but in reality, the vast majority of crystals have Fermi surfaces with shapes deviating from a sphere. What happens then to the electrons when they travel in a solid? In their trip they see Fermi surfaces which are like dance floors. On a floor full of obstacles like tables, chairs, pillars, and moreover is not flat, the electrons dance is hampered disturbing them to get into the next floor while on a nice flat empty one they will dance and progress coherently. Using STM, the fingerprints of their coherent dance can be observed.

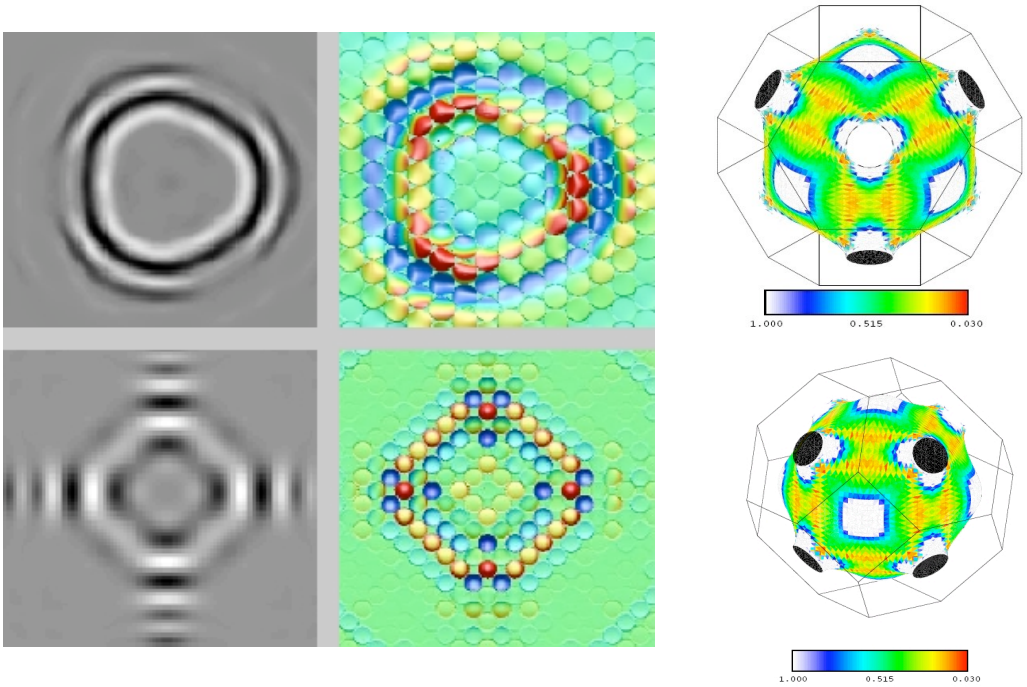

Figure 5: Electron ripples due to buried impurities below copper (111) surface (upper figures) and copper (001) surface (lower figures). The experimental measurements of Weismann and coworkers (University of Göttingen) in the left side are compared to Jülich's theoretical calculations in the middle for areas of 3nm x 3nm. The Fermi surface (right) for Cu is shown along the two directions 111 (upper) and 001 (lower). The red colors represent very flat surface regions and correspond to what is seen on the surface with STM.

For copper, the surface of Fermi is shown in Figure 5 (right) where the flat regions are colored in red. Their positions and their shape correspond to what is seen as oscillations on the surfaces along the two different directions.

Thus, besides detecting the buried objects, nanosonars can also be used to get information on the Fermi surfaces i.e. the dance floors and the roads that the electrons would use as well as other physical properties. The magnetic properties of the buried objects can also be grasped thanks to the different reflections experienced by the electrons if they hit a magnetic surface compared to non-magnetic surfaces. This is like throwing a ball against the wall or against a mattress. The reflection is not the same.

Summary:

Not every idea of Jules Verne became real! Futuristic excitement aside, there is this big dream of designing the world, the nanoworld, atom by atom, a world full of new phenomna, but this dream has to obey the laws of quantum mechanics and has to match the advances being made in nanotechnologies to become available to everybody. Frequently patience is required. However, scientists in Jülich while investigating the frustration of magnetic interactions and the dance floors and the roads of the Lilliputian quantum mechanical world of electrons, atoms and molecules invented two concepts realizable with actual technologies: Nanodominos and nanosonars. These can be the brains and the eyes of future nanites.

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References:

1 The simulations are based on density functional theory for which W. Kohn, was awarded the 1998 Nobel Prize in Chemistry.
2 The Korringa-Kohn-Rostoker Green function method is the simulation tool developed in Jülich.
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