From single constituents to correlation: phase transitions in few atom systems

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Abstract. The advancements of nanofabrication, together with the control of implantation of individual atoms at nanometric precision, have opened the experimental study of phase transitions of electronic systems constituted by six electrons and less. Here I review the recent advancements made in the field of phase transitions at the few atoms scale, including the discretized version of the Anderson-Mott quantum phase transition and the melting of electrons arranged in a Wigner-like phase into a Fermi glass realized in a $\text{Si}:X$ quantum device where $X$ is a donor element. The rise of collective phenomena is directly probed by controlling the distance between few donor atoms. Four atoms are sufficient to observe emergent phenomena such as Hubbard bands instead of single particle behaviour.

1. Introduction
The study of the Anderson-Mott transition [1, 2] have raised a considerable experimental and theoretical interest for decades.[3, 4] One of its manifestations, given by the transition from delocalized to localized electrons in semiconductors (a metal-insulator transition) triggered by the doping concentration by a different donor element, has represented a hard problem to solve theoretically and experimentally, even in the case of the most simple and well known case of doped silicon ($\text{Si}:X$ where $X = P, As$).[4] The possibilities opened by nanofabrication of semiconductor devices [5, 6] have been exploited by engineering the ability to control the position of impurity atoms at nanometric precision by a one-by-one method of implantation called single ion implantation (SII). Taking advantage of this method, developed in the last decade by three groups in the world [7, 8, 9], it has been possible to create chains of individually implanted ions in silicon [10], and to investigate the effects caused by their proximity and the residual disorder affecting their position and ground state energy distribution [11]. Therefore, the transition from a single particle behaviour to collective phenomena is directly observed. In the following, I recall the basic ingredients of the models involved in the Anderson-Mott transition, i. e. the Anderson transition and the Mott transition. Next, I describe the physics observed in single atom transistors, the band formation in arrays of donors, and finally the phase transitions observed in such systems. To conclude, only four elements are sufficient to exhibit the emergence [12] of a collective many-body behaviour.
2. Short review on metal insulator transitions

With metal-insulator transitions (MIT) are generally intended transitions of the electron states from delocalized to localized electron wavefunctions. MIT phase transitions are generated by means of two possible mechanisms: a structural change due to a change in the ionic lattice, or purely electronic. In this second case, two limiting cases are classified: Mott phase transitions, triggered by electron correlation and Anderson phase transitions, triggered by disorder. Transitions in which the competition of the two latter mechanisms concur, the transition is referred as Anderson-Mott transition. In the following we consider only the purely electronic phase transitions. The Mott transition is captured by the Hubbard Hamiltonian:

\[ H = t \sum_{\langle i,j \rangle} (a_{i\uparrow}^+ a_{j\uparrow} + a_{i\downarrow}^+ a_{j\downarrow}) + U \sum_i n_{i\uparrow} n_{i\downarrow} \]

where

\[ n_{i\sigma} = a_{i\sigma}^+ a_{i\sigma}, \]

\( t \) is the hopping matrix element and \( U \) is the on-site repulsion energy (\( U > 0 \)). The Anderson transition is governed by the Hamiltonian

\[ H = t \sum_{\langle i,j \rangle} a_{i\uparrow}^+ a_{j\uparrow} + \sum_i \epsilon_i a_{i\uparrow}^+ a_{i\uparrow} \]

which is a non-interacting electrons model, so spin here only provides a trivial factor of two which is omitted. The energies \( \epsilon_i \) are distributed within a bandwidth \( W \): Anderson predicted for \( W/t \) large but finite a transition from delocalized states to insulating regime. Delocalization is achieved by either decreasing the density of scatterers, or, for soft scattering potential, increasing energy of scattered particles. Pure Anderson transition is not expected to be realized in nature, as Coulomb interaction between electrons is always present. To describe the effects of the Anderson transition in semiconductors such as silicon in which disorder is introduced by the addition of donor atoms, such as P and As, the Mott transition, which would be inadequate if considered alone, has to be taken into account. Conclusion that has been reached over the years is that neither Andersons nor Motts picture itself is sufficient to understand the observed MIT in semiconductors[4]. The resulting quantum phase transition, which carries aspects of both types of transitions, is called an Anderson-Mott transition.

3. Single atom transistors

Single electron phenomena in defects have been originally observed in silicon/silicon oxide interfaces from random telegraph signal in small devices [13, 14, 15, 16, 17, 18]. Later, single electron effects have been observed in donor at the silicon/silicon oxide interface.[19] Individual atoms centered between the source and the drain of a small device provide the energy levels for sequential tunneling. The first observation of single impurities in silicon were obtained by using a small field effect transistor [19, 20] or a small flash memory [21] with a silicon channel, in which an impurity was randomly diffused from the doping of one of the contacts. The presence of the individual atom is observed by looking at the quantum transport of the device at cryogenic temperature [22, 23, 24]. The condition necessary to observe the quantum transport is that the overlap integral between the electron wavefunction and the conduction electron wavefunction exponentially decaying out of the doped region is sufficiently large so that the probability of creating sequential tunneling from the contact to the donor site and from the donor site to the second contact is measurable. Generally the host device, which is equipped with a top gate, at 4 K behaves as an electrostatic quantum dot (QD) in Coulomb blockade regime. The energy scale governing the Coulomb blockade oscillations in a QD is set by the charging energy.
$U = E_C + (E_{n+1} - E_n) = e^2/2C$, where $C$ is the total capacitance of the QD island relative to the surrounding conductors, $E_n$ is the energy of the $n^{th}$ level and $-e$ is the electron charge. If the single donor is positioned along the channel, it provides a second set of localized eigenstates of electrons corresponding to additional permitted energy levels below the conduction band edge. In Ref. [11] transistors fabricated on 100 silicon-on-insulator (SOI) substrates with 125-nm-thick buried oxide (BOX), which acts as a back-gate oxide, are considered. The nominal channel length is 200 nm, the width and thickness of the channel are 100 nm and 90 nm, respectively. Here only the Coulomb blockade of the atoms is observed, while no quantum dots are formed. The channels are in contact with highly doped n-type source and drain regions and are controlled by a gate bias ($V_g$) from the substrate through the buried oxide. The device exhibits accumulation-mode n-type transistor operation. The arsenic and phosphorous ions implanted two by two at 60 keV into the channel through the surface oxide with 10 nm thick are expected to distribute around the depth of 53 nm from the interface on the back side. Transistors with only two atoms implanted along the channel, for which their average distance is of the order of 20-40 nm, are treated as isolated particles. This is experimentally confirmed by looking at the quantum transport below the threshold voltage $V_T$ which probes the silicon band gap. There, Coulomb blockade is observed at low temperature (4-20 K). Coulomb blockade reveals that one electron occupies the ground state of each donor (first peak) and a second may occupy the second available state, as the charging energy is sufficiently low so that a second electron can stay bound to the donor (the $D^-$ state, which has a 5 times larger extension). To resume, in this regime the single particle behaviour is observed through the Coulomb blockade caused by two isolated donors which create two pairs of discrete energy levels in the band gap of the silicon.

4. Hubbard band formation in arrays of atoms in silicon

If one moves from the extremely dilute impurity concentration of previous paragraph, which is conventionally defined as $n < 1 \cdot 10^{16}$ cm$^{-3}$ in bulk silicon, such that $r_C > 46.4$ nm where $r_C = n^{-1/3}$, [25], to higher concentrations, one first achieves a linear density which corresponds to a cubic lattice density $n$ between $1 \cdot 10^{16}$ cm$^{-3}$ and $10^{17}$ cm$^{-3}$ (r$_C$ = 21.5 nm), called semidilute regime, characterised in bulk silicon by the formation of pairs and complexes because of the randomness of the donor distribution. At higher linear density, which corresponds to approximately $10^{17}$ cm$^{-3}$, Hubbard bands are formed (intermediate regime) with activation energies of $\varepsilon_2$ and $\varepsilon_3$ for the upper and lower bands, respectively, triggered by temperature. Such a classification has been created for bulk semiconductor. The novel single ion implanted quantum devices have shown that the Hubbard impurity bands are observed also for arrays of few atoms. This is observed experimentally as flat bands below the conduction band (the threshold voltage of the transistor) in I-V$_G$ characteristics (Figure 1, top-right). The number of atoms needed to create such bands is very small. Four and six atoms are sufficient to observe band formation. As each donor provides a double-spin-degenerate ground state that is also six-fold valley-degenerate, a system of 4 atoms has 48 available 1s states to create the band. Consequently the discretize version of the Anderson-Mott transition is observed by doubling the linear average density of the atoms in the device. In Figure 1 the formation of the Hubbard bands in a transistor of effective length of about 150 nm doped with an array of 4 atoms is reported as first derivative of the I-V$_G$ curves at many temperatures. The gate voltage $V_G$ scans the upper part of the silicon bandgap of the channel of the device. The conduction band edge is represented by the threshold voltage $V_T$. On the left, at low temperature, the contrast shows the Coulomb blockade transport through the localized energy levels provided by the four As donors. By increasing the temperature, the combination of the correlation and of the thermal activation determines the rise of the two partially overlapped Hubbard bands. As the frozen electron system is created at 4 K, we may call it a Wigner-like phase (each electron occupies a site of the potential landscape created by the 4 donors). By raising the temperature, the
Figure 1. Band formation in an array of 4 atoms below the threshold voltage $V_G$. From Ref. [11]. In region 1, the sequential tunneling through the array of 4 atoms energy levels dominates. By raising the temperature, the lower Hubbard band (2) and the upper Hubbard band (3) are formed.

electron system becomes better described in terms of Fermi glass.[2]

5. Conclusion
To conclude, recent experiments have shown that the emergence of phenomena typical of many-particle physics is possible with only four electrons confined thanks to an array of donors contained in a silicon quantum devices operated at cryogenic temperature. This kind of device opens the exploration of emergence at the nanoscale, when only few elementary constituents are employed and controlled.

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