Towards room temperature solid state quantum devices at the edge of quantum chaos for long-living quantum states

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Abstract. Long living coherent quantum states have been observed in biological systems up to room temperature. Light harvesting in chromophores is realized by excitonic systems living at the edge of quantum chaos, where energy level distribution becomes semi-Poissonian. On the other hand, artificial materials suffer the loss of coherence of quantum states in quantum information processing, but semiconductor materials are known to exhibit quantum chaotic conditions, so the exploitation of similar conditions are to be considered. The advancements of nanofabrication, together with the control of implantation of individual atoms at nanometric precision, may open the experimental study of such special regime at the edge of the phase transitions for the electronic systems obtained by implanting impurity atoms in a silicon transistor. Here I review the recent advancements made in the field of theoretical description of the light harvesting in biological system in its connection with phase transitions at the few atoms scale and how it would be possible to achieve transition point to quantum chaotic regime. Such mechanism may thus preserve quantum coherent states at room temperature in solid state devices, to be exploited for quantum information processing as well as dissipation-free quantum electronics.

1. Introduction
After the seminal observations of quantum coherence in biological systems in the last few years[1], a model has been developed for explaining such unpredicted phenomenon due to Vattay, Kauffman and Niiranen [2]. The protection of the coherence of quantum states in disordered systems is granted by the multifractality of wavefunction when delocalization starts to take place between insulating and disordered conductive regime. Doped silicon where impurity disorder occurs represents the ideal environment to create such conditions artificially.[3] The study of the Anderson-Mott transition from delocalized to localized electrons in semiconductors triggered by the doping concentration is a metal-insulator transition (MIT)[4, 5, 6, 7]. Such MIT 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 such as Si:As and Si:P.[7] The possibilities opened by nanofabrication of semiconductor devices [8, 9] consist in the control of 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 [10, 11, 12], it has been possible to create chains of individually implanted ions in silicon [13, 14], and to investigate the effects...
caused by their proximity and the residual disorder affecting their position and ground state energy distribution [15]. The transition from a single particle behavior to collective phenomena is directly observed. In the following, I review the recent advancements in the light harvesting biological systems, the physics observed in single atom transistors including the band formation in arrays of donors, and the key features of disordered doped semiconductors in the Anderson-Mott transition to emulate light harvesting systems where long-living quantum states may exist. A semi-Poisson edge of quantum chaos regime is predicted to exist in suitably deterministically doped [16] group IV semiconductor devices.

2. Anderson-Mott transition and disorder in doped semiconductors

In this section the metal-to-insulator transition generated by impurity doping in semiconductors such as silicon are considered. MIT phase transitions where the electron states evolve from delocalized to localized wavefunctions, 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 are referred as Anderson-Mott transition. To start, let’s first consider the purely electronic phase transitions. The Mott transition is captured by the Hubbard Hamiltonian:

\[ H = t \sum_{\langle i,j \rangle} (a^+_i \sigma a^\downarrow_j \sigma + a^\downarrow_i \sigma a^+_j \sigma) + U \sum_i n_i \sigma n_i \sigma \quad (1) \]

where

\[ n_{i\sigma} = a^\dagger_{i\sigma} a_{i\sigma}, \quad (2) \]

\( t \) is the hopping matrix element and \( U \) is the on-site repulsion energy (\( U > 0 \)). Though, impurity doping in semiconductors induces disorder, which in turn is captured by the Anderson transition governed by the Hamiltonian

\[ H = t \sum_{\langle i,j \rangle} a^\dagger_i a_j + \sum_i \epsilon_i a^\dagger_i a_i \quad (3) \]

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. Neither Anderson’s nor Mott’s picture itself are sufficient separately to understand the observed MIT in semiconductors[7]. The resulting quantum phase transition, which carries aspects of both types of transitions, is called an Anderson-Mott transition.

3. Quantum chaos in disordered semiconductors

Manifestation of quantum chaos has been investigated in the nineties [3], by revealing a rich variety of different regimes. Let us first recall that discrimination among integrable and chaotic system is reflected in the level spacing distribution \( P(s) \) where the spacings \( s \) of neighboring energy levels differs depending on the regime of the system: the energy levels of integrable
systems are not correlated, and not prohibited from crossing, so their distribution is Poissonian (P):
\[ P_P(s) = e^{-s} \] (4)
while in chaotic systems the eigenvalues become correlated and crossings are avoided, which determines level repulsion, so their distribution is described by the Wigner-Dyson (WD) distribution,
\[ P_{WD}(s) = \frac{\pi s e^{-\pi s^2/4}}{2} \] (5)
as predicted by random matrix theory. The form of the Wigner-Dyson distribution depends on the symmetry properties of the Hamiltonian. Time reversal invariance imply a Gaussian orthogonal ensemble (GOE). The edge between the two regimes where the transition between the two regimes occur and where the wavefunction of the system becomes multifractal is described by the semi-Poisson distribution (SP):
\[ P_{SP}(s) = 4s e^{-2s} \] (6)
The latter is the regime where long-living quantum states may exist. Band structure calculations reveal that crystalline materials unambiguously manifest quantum chaos. Silicon can be seen as a quantum chaotic system with a particularly simple diatomic unit cell and the false time-reversal violation carries GOE distribution in the entire Brillouin zone away from symmetry points, described by
\[ P_{GOE}(s) \propto s e^{-\pi s^2/4} \] (7)
On the contrary, alloy III-V semiconductors such as AlGaAs lack of inversion symmetry of the unit cell to T is broken outside the Γ point and the ensemble is unitary (GUE). The latter is expressed as:
\[ P_{GUE}(s) \propto s^2 e^{-4s^2/\pi} \] (8)
being generated by unitary instead of orthogonal random matrix ensemble. Simulation show that in the proximity of the symmetry points the band distribution is Poissonian, while away from such points is GOE in silicon.

4. Experiment with few atom transistors
Single electron phenomena in defects have been originally observed in silicon/silicon oxide interfaces from random telegraph signal in small devices [17, 18, 19, 20, 21, 22]. Later, single electron effects have been observed in donor at the silicon/silicon oxide interface.[23] Individual atoms centered between the source and the drain of a small device provide the energy levels for sequential tunneling, 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 [24, 25, 26]. 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. When the single donor is positioned along the channel, it provides a set of localized eigenstates of electrons corresponding to permitted energy levels below the conduction band edge. In Ref. [15] 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. The arsenic and phosphorous ions implanted two by two at 60 keV into the channel through the surface oxide with 10nm 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 $V_G$ which probes the silicon band gap, which shows Coulomb blockade at cryogenic temperature. When one moves from such an extremely dilute impurity concentration, which is conventionally defined as $n < 1 \cdot 10^{16}$ cm$^{-3}$ in bulk silicon, such that $r_C > 64.4$ nm where $r_C = n^{-1/3},$ 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, characterized 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 $\epsilon_2$ and $\epsilon_3$ for the upper and lower bands, respectively, triggered by temperature. The Hubbard impurity bands are observed also for arrays of few atoms as flat bands below the conduction band. The number of atoms needed to create such bands is very small. Four and six atoms are sufficient to observe band formation. By increasing the temperature from base 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 electron system is described as a Fermi glass.[5]

5. Discussion: application of deterministic doping towards the edge of quantum chaos in silicon quantum devices

The combination of the concepts reviewed in the previous sections opens novel scenarios of capital interest for solid state quantum information. The discovery of the mechanism enabling nature to preserve the quantum coherence at longer timescales thanks to the special properties of multifractal systems suggest a method for extending quantum coherence in quantum devices where fast decoherence proved to be a major issue. Such issue is technologically so severe that currently, after almost 20 years of development of solid state quantum information devices, tuning four qubits for circuitual quantum information represents the maximum success, while at least 1000-10000 qubits are needed to implement quantum error correction codes. The special properties in the multifractal regime at the edge of quantum chaos consist in the simultaneous realization of sufficiently extended delocalization of wavefunction, together with power law decay of the coherence instead of exponentially fast loss of coherence of delocalized systems. In order to exploit the lesson learned from nature in the light harvesting systems, which display long-living quantum states up to room temperature thanks to a sort of lucky low-dissipation energy state distribution, and to apply to quantum information solid state devices, one may exploit a controlled quantum transition in semiconductor energy bands. Group IV semiconductors such as silicon and germanium are considered suitable for the long coherence times permitted by the lack of spin-orbit interaction, which on the contrary affects III-V semiconductor quantum devices. Group IV semiconductor bands engineering from undoped to impurity doping condition naturally carries the transition across the edge of quantum chaos. Indeed, if one consider high symmetry points such as $\Gamma$ point for holes in undoped silicon and both electrons and holes in germanium, as well as $X$ point for electrons in silicon, the energy spacing distribution is Poisson-like.[3] At the same time, doping is able to move the system to a GUE condition with no need to move away from such symmetry point, by gradually increasing the degree of disorder with the employment of deterministic doping method. Such an aspect represents the key fact of tuning the transition from Poisson to semi-Poisson condition, i.e. the chance to maintain the carriers within the same point in reciprocal space where conduction already takes place. According to what observed in biological light harvesting systems, where exciton states live for unexpectedly long times even at room temperature, we may expect that a similar behaviour may arise in
quantum states living in suitably doped group IV semiconductors. Single ion implantation can therefore play a major role to implement the designed doping in realistic solid state quantum devices created to coherently transfer quantum information.

6. Conclusion

To conclude, recent experiments have shown that the long-living coherent quantum states may exist up to room temperature in biological systems thanks to quantum chaos. Such phenomenon may in principle be swapped in doped semiconductors, where a high degree of control down to single atom control at nanometric precision has been proved. The combination of quantum chaos with doped semiconductor physics may lead to long-living quantum states to be exploited for quantum information processing as well as dissipationless quantum electronics.

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