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Single spin electron spin resonance (ESR) using scanning tunneling microscope (STM): sensors and qubits.

1. **A quantum sensor for atomic-scale electric and magnetic fields**
   Authors: Taner Esat, Dmitriy Borodin, Jeongmin Oh, Andreas J. Heinrich, F. Stefan Tautz, Yujeong Bae, Ruslan Temirov,
   arXiv to appear.(Preprint is available upon rquest from the authors. Contact heinrich.andreas@qns.science)
2. **An atomic-scale multi-qubit platform**
   Authors: Yu Wang, Yi Chen1, Hong T. Bui, Christoph Wolf, Masahiro Haze, Cristina Mier, Jinkyung Kim, Deung-Jang Choi, Christopher P. Lutz, Yujeong Bae, Soo-hyon Phark, Andreas J. Heinrich,
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Recommended with a Commentary by Patrick A. Lee, MIT

The observation of electron spin resonance signal from a single atom using an STM tip was realized in 2015 [1] and considerable progress has been made since that time. (For additional references see the recommended papers). The two recommended recent papers report particularly striking advances which should be of interest to the condensed matter as well as the quantum computing community. In the first paper, a molecule carrying S=1/2 is attached to an STM tip and a sharp electron spin resonance is observed. The shift of this resonance can be used for the sensing of very small magnetic field and electric field, with angstrom scale spatial resolution. The second paper reports the use of the ESR signal of a sensor atom located on a surface to interrogate two other S=1/2 atoms which serve at qubits. Remarkable coherence properties and two qubit operations are demonstrated using pulsed fields techniques. This commentary will focus mostly on the first paper, with a brief discussion of the second paper at the end.

A better known system that displays ESR at the single ion level is the NV center in diamond.[2] The very narrow resonance of the NV center can be used to measure local magnetic fields down to micro-Tesla $Hz^{1/2}$. By placing the diamond on an AFM tip, scanning is also possible. However, since the NV centers are located on the scale of tens of nanometers from the surface, this limits the distance of NV center from its target and therefore the spatial resolution to tens of nanometers. On the other hand, the vertical position of the tip can be varied which raises the possibility to measure the fluctuation spectrum of the magnetic field as a function of distance. The information on the magnetic fluctuation spectrum of the substrate can be measured via the T_1 of the spin, at a frequency giving by the level spitting which can be controlled by a magnetic field. The dependence on the vertical position gives information about the q dependence. It has been proposed that this may serve as a kind of poor man's neutron scattering with the caveat that the q resolution is limited to the inverse of tens of nanometers. [3].

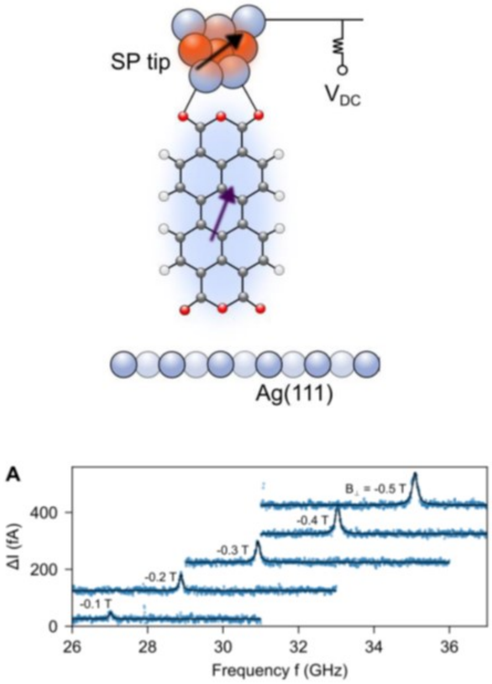

Figure 1: Top panel shows the ESR/STM set-up. Several Fe atoms are picked up by a Ag STM tip to form a spin polarized tip. An organic molecule (PCDTA) which contains spin 1/2 is then picked up. The assembly forms a scanning tip over a Ag(111) substrate. An AC voltage is applied to drive the spin resonance of the molecule. The resonance signal is detected by the DC tunneling current, due to magnetoresistance of the spin polarized tip. Bottom panel shows the ESR spectrum obtained by scanning the frequency of the AC field for several values of B field applied roughly perpendicular to the plane .

For NV centers the spin state is excited by a microwave field which drives the resonance and is detected optically by the luminescence from an optically pumped level. In contrast, for ESR-STM, the drive is accomplished by modulating the voltage between the tip and substrate. With appropriate spin orbit coupling of the magnetic atom, the AC electric field has a magnetic component which drives the resonance. Detection is accomplished by using a spin polarized tip : the magnetic state of the spin is detected by measuring the tunneling current, which depends on the magnetization of the sensor atom or molecule via a magnetoresistance effect. This scheme was demonstrated for an atom adsorbed on a surface.[1] In that case it is necessary to place an insulating layer on top of a Ag substrate. Otherwise, because the spin is so close to a metal, the magnetic fluctuations from the metal broaden the resonance line to make it un-observable. In the new development, a spin polarized tip is first prepared by attaching a few Fe atoms to a Ag tip. After that an organic molecule containing an S=1/2 spin state (PTCDA) is picked up from the surface and acts as a sensor. The spin resonance is observed by modulating the voltage and measuring DC tunneling current as before. An example of the spin resonance is shown in Fig. 1. The line-width is about 0.1 GHz which means that a frequency shift of a fraction of that can be measured. This corresponds to an energy resolution of 100 nV or a magnetic field of 4 gauss. The authors make the point that unlike equilibrium measurements, in resonance experiments the resolution is not limited by the thermal energy kT, but by the resonance width which is much smaller. The data shown in Fig. 1 is taken at 1.4K and currently the temperature range is between mK and 5K. The upper limit is much lower than that of the NV center due to technical reasons related to the excitation scheme.

There is a complication that the Fe atoms on the tip produce an exchange field which needs to be determined because the ESR frequency is sensitive to the vector sum of the exchange field and the external field. Paper 1 shows this can be done by fitting the spectra for two orientations of the applied fields. Once the exchange field is known, the molecule is now a mobile scanning sensor of magnetic field with the angstrom resolution of the STM tip. The spin is typically located about 15 angstrom from the surface which sets a limit of its resolution if spatial averaging is involved. It turns out that the ESR line is also sensitive to a local electric field, presumably because it shifts the position of the bonding electrons and affect the environment of the spin state. Paper 1 demonstrate that that the dipolar magnetic field due to local spin 3/2 moment of an Fe atom as well as the electric field due the dipole moment of a Ag dimer on the surface can be measured.

The ESR/STM system creates an entirely new capability of local electric and magnetic field sensing at the atomic scale which is not available before, and the readers are invited to use their own imagination to daydream about possible applications. My list includes sensing of the fringe magnetic field above a spin density wave (SDW) which may arise in monolayer or twisted TMD's. For example, it is suspected that the super-modulation observed in 1T-TaSe2 may be a $2k_F$ SDW.[4] Also antiferromagnetic order may be detectable in moire graphene and TMD's that exhibit Mott transitions.[5, 6] These structures require a dual gate set-up, and perhaps the fringing magnetic field above the sample can be detected if the top gate is sufficiently thin. On the other hand, since the detection scheme requires a tunneling current, the vertical distance cannot be varied much which means that while the magnetic field fluctuation spectrum can be detected via the T_1 of the spin state, this can only be done at a fixed distance, and lack the q information available with NV centers described above. Nevertheless, even this fixed position spectrum can be of interest in special cases. One example is the detection of magnetic field fluctuations above a spin liquid with a spinon Fermi surface.[7]

Before we get too carried away, it should be noted that paper 1 points out that so far the success rate of producing an operational sensor out of the fabricated tip is about 5 percent. So perhaps further developments will be warranted.

Let me briefly mention a second development which reveals the coherence properties of the spins and their potential use as qubits. In this set-up a sensor Ti atom is deposited on an insulator coated surface and two other Ti atoms are deposited about 10 angstrom away.

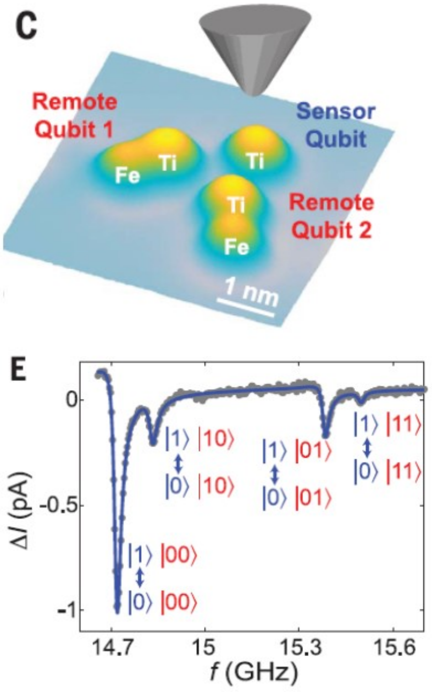

Figure 2: Top panel shows a spin polarize STM tip tunneling to a Ti atom which contains S=1/2 and serves as the sensor qubit. Two other Ti atoms serve as qubits 1 and 2. The only role of the Fe atoms is to convert the electric field of the AC drive to a magnetic field which can excite the spin resonance. As long as the qubits are located within 10 nm of the tip, they can be resonantly excited and manipulated. Lower panel shows the ESR spectrum of the sensor qubit. The 4 lines correspond to 4 possible configurations of the two qubits . The are labeled by the Ket states of the spins.

Due to dipolar coupling between the spins, the resonance energy of the sensor spin depends on the spin state of the other two spins. As a result, 4 lines are resolved which depends on the 4 possible spin states of the target spins which will serve as qubits. (see fig. 2.) Using pulsed field techniques, the target spin states can be manipulated over the Bloch sphere in the standard way. Notably, there is no tunneling current through the qubits: the qubits are measured via the sensor qubit only. Using the fact that the resonance frequency assigned to qubit 1 is conditioned on the state of qubit 2, a CNOT gate was demonstrated. Presumably these impressive results can be extended to a few more qubits, but further scaling up appears to be difficult because the qubits must be located within about 10 angstrom of the sensor qubit to have a large enough coupling to the AC drive as well as sufficient coupling to the other qubits.

These recent developments show that ESR/STM has the sensitivity, spatial resolution and coherence properties which are unique and this system may be poised to gain popularity and further exploitations.

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