Erio Tosatti

Current Research Interests

1. Nanofriction theory and simulation
   Building on prior surface science expertise, I develop theory and simulation to understand mechanical friction -- and also electronic and magnetic dissipation -- initially of nanosized sliders and tips on solid surfaces. Once obtained, that insight, of value on its own merit, should also serve additional purposes. First, the complex multicontact stick-slip sliding processes typical of mesoscale and macroscale friction can be better addressed based on the single contact understanding obtained. Second, fundamental theory of friction, rather scarce so far on account of the nonlinear and generally violent dynamics involved, could be better developed and tested beginning at the atomistic level typical of the nanoscale.
   In my group we deal with all these aspects, inspired by recent techniques and data, and using theory and molecular dynamics simulation as tools to make progress.

2. Theory of metallic and magnetic nanocontacts, especially of Kondo transport anomalies. Metallic nanocontacts, realized by mechanical break junctions, or by electromigration, or by a tip approaching a surface, possess interesting structural, mechanical and electronic properties. Their electrical conductance is ballistic, entirely ruled by quantum mechanics as opposed to Ohm's law of ordinary conductors. Magnetism affects the electronic structure and thus the spin polarized conductance. A magnetic impurity in a nonmagnetic contact undergoes Kondo screening, whose nature and magnitude is directly revealed by so called zero bias conductance anomalies. A quantitative theoretical approach to this Kondo phenomenon is only possible by implementing schemes that could at the same time describe the nanocontact electronic structure from first principles (such as DFT) and the many body physics typical of the Anderson model (such as NRG). Lacking a reliable scheme simultaneously covering both aspects, in my group we use a DFT+NRG scheme, where first principles and Anderson models are piecewise joined together. Besides regular Kondo, potential cases of so called ferromagnetic Kondo are presently under scrutiny.

3. Mott insulating and unconventional superconducting states of fullerides and molecular conductors
   There are families of molecular conductors built by doping with alkali atoms such as K, Rb, Cs molecular crystals that were initially insulating such as fullerene, polycyclic aromatic hydrocarbons, and others. Interestingly, superconductivity arises quite commonly in these doped systems, with temperatures that may exceed 30 K in the case of fullerides. Electrons donated by the alkali occupy a molecular LUMO derived band, which is generally narrow enough to suggest that electron correlations may be very strong, so the simple metal picture necessary for a BCS description may be invalid. In my group we have developed the view, based on calculations and models, that fullerides, especially the most expanded ones, are strongly correlated. In fact, our
models suggest that superconductivity, although driven by vibrations like BCS, arises here as a direct consequence of a nearby Mott metal insulator transition, and is quite different from BCS. Recent data on the new material Cs3C60 fully confirm the predictions of this model. Finding out whether strong correlation physics is relevant or not to the other doped molecular superconductors is an open challenge, which is the subject of current work.

4. Strong electron correlations and phase transitions at surfaces

The surfaces of semiconductors offer a physically unique situation, where the broken surface bonds give rise to very narrow two-dimensional "dangling bond" electronic bands in the middle of the underlying three-dimensional insulating bulk energy gap. Half filled, this bands would give rise to a two-dimensional metal -- a situation that is however highly unstable. In the first place, this ideal surface is highly reactive, and will easily become passivated, either by extrinsically, by reactions with outside chemicals, or else intrinsically, by spontaneous "reconstruction" of the surface atomic positions. In some cases, however rare, passivation or reconstruction can be averted, and the physics of a very narrow and strongly correlated band can appear. Such is the case, for example, of Sn/Si(111) at one third coverage. In this case, tunneling spectroscopy shows a metallic state of the surface at room temperature, turning to an insulating state at low temperatures, which in all probability is a Mott insulator. The challenge here is to understand how it could be possible, by doping or otherwise, to transform the surface away from this parent insulating state, possibly to a two-dimensional d-wave superconducting state, akin to that of cuprates.

5. Physics of ultra-high pressures

At pressures around one megabar, condensed matter looks very different indeed. Many molecules dissociate and phase separate into the atomic constituents; or else they give rise to new unprecedented compounds. For example, CO2 turns from a soft molecular crystal into a hard, piezoelectric crystal similar to SiO2, quartz. Packing increases, and insulators tend to become metals, often superconductors. Magnetism disappears, and the narrow bands of a transition metal such as iron may broaden out to mimic those of a simple metal like aluminum. The variety of possible behavior under pressure is unpredictable by simple common sense. While the higher and higher pressure diamond anvil cell experiments that progressively unveil this variety are getting increasingly difficult and costly, calculations and simulations are getting comparably easier, as the accuracy of the DFT approximations used for ab initio simulations and calculations increases for increasing density. For many systems it is now becoming not just more economical, but probably more reliable too to pursue ultra-high pressure phases by ab initio molecular dynamics than by actual experiments. The simulation method in use by my collaborators is a merger of the Parrinello-Rahman and Car-Parrinello techniques, where atoms enjoy a lot of freedom to arrange and rearrange in the lowest free energy state as pressure is cranked up. With this type of simulations much more is still open for discovery.

6. Quantum paraelectrics

In a classical displacive ferroelectric, for example in perovskites such as BaTiO3, the oxygen cage surrounding the central Ti ion is too large, and the Ti atom "falls" on one of six equivalent sides. The distortion thus generated transmits to the next cage, so that the next Ti ion also falls on the same side. In the end, the resulting overall ground state has all Ti ions displaced off center along the same direction, which gives rise to the macroscopic dielectric polarization called ferroelectricity. When however the off center "displacive" distortion is very small, quantum mechanics plays a role, and starts a new game. Quantum mechanics tries to tunnel each Ti ion
from one to another of the six equivalent sides. When this quantum perturbation is strong enough, it destroys order altogether, turning the ferroelectric into a "quantum paraelectric": the ferroelectric state has undergone quantum melting. Such is the state of affairs in SrTiO3, and to some extent also of KTaO3. This is a suggestive situation, perhaps because so many other quantum melted states possess "super" properties, sometimes referred to as off-diagonal long range order. Helium crystal turns superfluid, charge-density waves turn superconducting, etc. Even 2D Wigner lattices turn into Laughlin states, which are not superfluid but are very remarkable indeed. Quantum paraelectrics can be assimilated to the Ising model in a transverse field, which has a quantum phase transition but no off diagonal long range order and indeed nothing remarkable. It remains to be seen if this is actually the final word.

Education

1967      Degree in Physics, University of Modena, cum Laude
1970      Doctorate in Physics, Scuola Normale Superiore Pisa, Magna cum Laude.

Positions held

1971-76          CNR Researcher, University of Rome “La Sapienza”, Rome, I
1972-73          Royal Society/NATO Fellow, Cavendish Laboratory, Cambridge, UK
1974               DFG Stipendium, University of Stuttgart, Germany
1977               Senior NATO Fellow, Stanford University, USA
1977-80          CNR Researcher and Physics Lecturer, University of Trieste, I
1980-2008      Founder and Head, Condensed Matter Theory Group, Int’l School for Advanced Studies (SISSA), Trieste, I
1984-85          Visiting Scientist,IBM Zurich Research Center, Rueschlikon, CH
2002-03          Acting Director, and Deputy Director (D-2), Abdus Salam Int’l Centre for Theoretical Physics (ICTP), Trieste, I
1977-now         Co-founder and Head, now Deputy Head, Condensed Matter Group, Abdus Salam Int’l Centre for Theoretical Physics (ICTP), Trieste, I
1980-now       Professor, Int’l School For Advanced Studies (SISSA), Trieste, I

Memberships

Italian Physical Society
European Physical Society
American Physical Society (Fellow, and life member)

Honors and Achievements

The Francesco Somaini Triennial Physics Prize, Como, 1997
Fellow of the American Physical Society, 2001
Tate Medal for International Leadership in Physics, American Institute of Physics, Washington D.C., 2005
Corresponding Member, Accademia Nazionale dei Lincei, Rome, 2006
Foreign Associate Member, U.S. National Academy of Sciences, 2011
ERC Advanced Grant awardee, European Union. 2012

Other Recognitions
Lamina Aurea di Redu', Nonantola, 1999
"Modenese di Peso", Museo della Bilancia, Campogalliano, 2009
ITIS "Fermo Corni" Prize and Lecture, Modena, 2009
"Ragno d'Oro" Prize, University and City of Modena, 2012

Named Lectures
The Eli Burstein Lecture Award, University of Pennsylvania, Philadelphia, 1994
The Alessandro Volta Medal and Lecture, University of Pavia, 2011
The Enrico Fermi Colloquium, LENS, Florence, 2011

Publications and Impact
Books (including Edited) 12
Articles and Review Articles in journals and books ~ 480
Total Citations (ISI Web of Science) ~ 12,000
Hirsch index H (H papers with more than H citations) ~ 60
m-index = H/years after PhD 1.4
PhD Students Supervised 1981-2011 32