ESF PESC EXPLORATORY WORKSHOP

Mott's Physics in Nanowires and Quantum Dots

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1 Current-controlled polaronic switching of molecular quantum dots

Sasha Alexandrov

Department of Physics, Loughborough University, Loughborough LE11 3TU, UK

a.s.alexandrov@lboro.ac.uk

The mechanisms of molecular switching and transport through molecular nanowires and quantum dots are of the highest current experimental and theoretical value. We have developed the multi-polaron theory of correlated transport through molecular nanowires and quantum dots (MQD) taking into account polaron-polaron correlations [1]. Attractive polaron-polaron correlations lead to a "switching" phenomenon in the current-voltage characteristics of MQD. The degenerate MQD with strong electron-vibron coupling shows a hysteretic volatile memory if the degeneracy of a molecular level is larger than two. The hysteretic behaviour strongly depends on the electron-vibron coupling and characteristic vibron frequencies. The current bistability vanishes above some critical temperature. Among potential candidates for the negative-U switching phenomenon are C_{60} molecules, where the electron-vibron coupling proved to be particularly strong, and other carbon nanostructures including short nanotubes.

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2 Manifestation of additional dimensions of space-time in semiconductor quantum dots

Alexander Andreev

P L Kapitza Institute for Physical Problems, Kosygin Street 2, 119334 Moscow, Russia

andreev@kapitza.ras.ru

1. Wick-Wightman-Wigner (3W) superselection rule.
2. 3W-rule and the existence of additional spinor dimensions of space-time.
3. Demonstration of the reality of additional dimensions in the experiment with the semiconductor double quantum dot.
4. Possible physical sense of additional dimensions for nonrelativistic systems.

3 Ultrafast polaron transport in biosystems

Serge Aubry

Laboratoire Léon Brillouin, CEA Saclay, 911191 Gif-sur-Yvette, France

saubry@dsm-mail.saclay.cea.fr

Enzymes (and many other biomolecules) are proteins (polymers of charged aminoacids) wrapped in a special conformation for reaching their functionality. For that reason, such systems are especially favourable to the formation of small adiabatic polarons since an extra electron should strongly interact with the charged radicals of its highly deformable environment and self-trap. Polarons in biosystems are associated with quite large local atomic reorganizations (and energy barriers). This is implicitly taken into account by standard chemical models describing electron transfer (ET) between a donor and an acceptor site (or molecule) as the consequence of a (generally) large thermal activation over the (polaronic) energy barrier. However, there are many biosystems which precisely gain their high efficiency and selectivity from ultrafast ET (at the scale of ps).

We shall propose nonlinear mechanisms for polaron mobility. In our first model (for the Photosynthetic Reaction Center), an electron transfer initially occurs by a reversible targeted transfer from the donor toward an extra catalytic site (which has to be specifically well tuned with the donor). Before ET to the catalyst is completed, a resonance with the acceptor is caught, so that ET is redirected (now irreversibly) to the acceptor. In that case, the energy barrier has been removed by a turn-around pathway via the catalyst.

A second model concerns signal transmission in allosteric enzymes such as ATCase. The regulation of this large enzyme is done by a few kinds of heavily charged but small molecules which bind at specific sites at its periphery. They can induce a drastic change of the local conformation of the far distant active site of the enzyme which opens or closes then switching the enzyme from inactive to active (or the reverse depending on the kind of bound molecules). We suggest that such a signal transmission may be obtained electromechanically by a mobile polaron pre-existing in the enzyme. It has different equilibrium locations depending on the electric field generated by the signs and the distribution of the charges of the bound molecules. We demonstrate a simple model showing that in principle, we may have barrierless and mobile polarons in non-periodic networks, providing the model parameters (also involving the electrostatic energies) are appropriately and finely tuned.

Similar polaron models could be suggested for other bioprocesses involving important conformational changes, for example for biomotors.

4 Ferromagnetic nanorings

Tony Bland, C A F Vaz, T J Hayward, J Llandro, F. Schackert, F Castano, D Morecroft, C Ross, M Klaeui, U Rudiger and G Faini

Cavendish Laboratory, University of Cambridge, JJ Thomson Ave, Cambridge CB3 0HE, UK

jacb1@phy.cam.ac.uk

Ferromagnetic metal rings of nanometre range widths and thicknesses exhibit fundamentally new spin states, switching behaviour and spin dynamics which can be precisely controlled via geometry, material composition and applied field. Electron transport provides an exquisitely sensitive probe of the presence, spatial location and motion of domain walls which determine the magnetic state in individual rings while magneto-optical measurements with high spatial resolution can be used to probe the switching behaviour of ring structures with very high sensitivity. Following the discovery of the 'onion state' which mediates the vortex switching [1], a range of fascinating phenomena have been found in these structures. For example we first show how the geometric parameters of ring elements determine the exact equilibrium spin configuration of the domain walls of rings in the 'onion state', and we show how such behaviour can be understood as the result of the competition between the exchange and magnetostatic energy terms [2–7]. The next example will be drawn from our studies of the displacement of domain walls by electric currents. By directly imaging the detailed spin structure and/or the position of domains walls following the application of a pulsed current, we are able to study the effect of spin currents on the wall velocities and on the domain wall structure itself [8–11]. Finally we show that magnetoresistance measurements can be used to explore stochastic switching events.

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5 Conductance through coupled quantum dots

Janez Bonča, R Žitko, A Ramšak and T Rejec

J Stefan Institute and Faculty of Mathematics and Physics, University of Ljubljana, Jadranska 19, 1000 Ljubljana, Slovenia

janez.bonca@ijs.si

Using three supplementary numerical methods: a) quantum Monte Carlo algorithm based on the constrained path method, b) variational approach, and c) numerical renormalization group technique we compute zero-temperature conductance through different interacting regions. We first test all methods on a single quantum dot system coupled to the leads. Comparison of our results with those obtained with the essentially exact Bethe ansatz method reveals excellent agreement. We then extend our calculations to three quantum dots coupled in series as well as to multiple quantum dot systems coupled in parallel. In the first case we study the effect of various strengths of inter-dot overlap on the shape of Kondo plateaus that appear as a function of the gate voltage. Our results for conductance are further supplemented with calculations of various correlation functions in terms of the gate voltage [1]. We also present the phase diagram containing different Kondo regimes. For the case of the side-coupled double quantum dot we present the evolution of the spectral function vs. gate voltage in different regimes of the inter-dot coupling strength [2].

In the second part of the talk we investigate several (N) quantum dots coupled in parallel to the same single-mode conduction channel. Using the generalized Schrieffer-Wolff transformation we show that near the particle-hole symmetric point, the effective Hamiltonian in the local moment regime is the N-impurity $S = 1/2$ Kondo model. This claim is further supported by comparing accurate numerical renormalization group results for magnetic susceptibility of the $N-$impurity Anderson model to the exact Bethe-Ansatz results of a $S = N/2$ $SU(2)$ Kondo system. Moreover, the Kondo temperature is independent of the number of impurities N. We demonstrate the robustness of the spin $N/2$ ground state by studying the stability of the system with respect to various experimentally relevant perturbations.

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6 Nano-structuring cuprate superconductors

Ivan Bozovic

Condensed Matter Physics and Materials Science, Brookhaven National Laboratory, Upton, NY 11973, USA

bozovic@bnl.gov

Using the "next-generation" molecular beam epitaxy system, we have reproducibly synthesized thin films of LaSrCuO, BiSrCaCuO and BaKBiO with rms surface roughness in the range $0.2 - 0.5$ nm. This technology has enabled fabrication of precise and uniform multilayers and superlattices, some of which contain barriers or HTS layers that are just one-unit-cell thick and yet have no pinholes over macroscopic areas. In turn, such heterostructures enable novel experiments that probe into the basic physics of HTS.[1-4]

In this talk, we will present our most recent results with such cuprate and bismuthate heterostructures, including XRD, AFM, RHEED, TOF-ISARS, LEEM, high-resolution TEM, transport, Hall effect, high magnetic fields (33 T), photo-induced absorption spectroscopy, photoconductivity, and resonant (synchrotron) X-ray scattering. We will also report on attempts to fabricate HTS nanowires and other nano-structures.

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This work has been done in collaboration with G Logvenov, V Butko, A Gozar, A Bollinger, Y Zhu, J.He, P Sutter (BNL); N Bozovic (SJSU), P Abbamonte (UIUC); G Boebinger, S Riggs (NHFML); F Balakirev (LANL); S Djordevic (Akron), and J Clahyhold (Miami U.)

7 Electron transport in nanostructures, including molecular quantum dots

Alex Bratkovsky

Hewlett-Packard Laboratories, 1501 Page Mill Road, Palo Alto, CA 94304, USA

alex.bratkovski@hp.com

A few molecular scale devices are reviewed here on the basis of first-principles and model approaches. Current rectification by molecular quantum dots can produce the rectification ratio 100. Current switching due to conformational changes in the molecules is slow, on the order of a few kHz. Fast switching THz may be achieved, at least in principle, in a molecular quantum dot with strong coupling with vibrational excitations. Defects in molecular films result in spurious peaks in conductance, apparent negative differential resistance, and may also lead to unusual temperature and bias dependence of current. The observed switching in many cases is extrinsic, caused by changes in molecule-electrode geometry, molecule reconfiguration, or metallic filament formation through the film. We also review some relevant experimental data that suggests a spurious/intermittent character of observed negative differential resistance in molecular devices. If time permits, peculiarities of spin transport in nanodevices will be briefly discussed.

8 Quantum statistics for a finite number of polarons in a quantum dot

Fons Brosens, S N Klimin, J T Devreese

TFVS – University of Antwerpen, Groenenborgerlaan 171, 2020 Antwerpen, Belgium

fons.brosens@ua.ac.be

The ground state energy of an N-polaron system confined to a quantum dot with a neutralizing background charge is investigated within an all-coupling many-body path-integral variational principle taking into account both Fermi statistics of polarons and the electron-electron interaction. The treatment of the ground-state energy is performed for both closed-shell and open-shell systems. The electron-phonon contribution to the ground-state energy as a function of the number of fermions demonstrates a trend to a constant value when increasing N. For a finite number of polarons, the dependencies of the ground-state energy and of the polaron contribution on the parameter r_s^*, which determines the average fermion density in a quantum dot, are very similar to those for a polaron gas in bulk. Herefrom, we can conclude that the ground-state properties of a polaron gas in bulk can be qualitatively described using a model of a finite number of polarons in a confinement potential provided by a background charge.

9 Correlated electrons and transport in nanostructures

Bogdan R Bułka[1], T Kostyrko[2], M Tolea[3] and I V Dinu[1,3]

[1]Institute of Molecular Physics, Polish Academy of Sciences, M. Smoluchowskiego 17, 60-179 Poznań, Poland
[2]Institute of Physics, A. Mickiewicz University, ul. Umultowska 85, 61-614 Poznań, Poland
[3]National Institute of Materials Physics, POBox MG7, Bucharest-Magurele, Romania

bulka@ifmpan.poznan.pl

We present our recent results on the role of electronic correlations in transport through nanostructures. First, we consider electronic transport through a quantum point contact (QPC) with an impurity site, which can accumulate a charge. Our model is a system of short coupled chains with a single impurity, described by the single-impurity Anderson Hamiltonian. The conductance is determined by means of the non-equilibrium Green-functions calculated by the equation of motion method. Most recent theoretical studies of QPC are confined to the Hartree-Fock approximation, which gives a solution with a local magnetic moment. However, this solution is not satisfactory because it corresponds to breaking a local symmetry of the Hamiltonian and it is in conflict with rigorously established theorems with a singlet solution. In our studies the Hubbard I approximation is used, which is reliable in a high temperature regime. For a low-dimensional system an impurity state lies below the band and the conductance shows a resonant transmission. However, due to the accumulated charge the conductance $\mathcal{G}$ is lowered to the value $(2/3) \times (2e^2/h)$. When the gate voltage increases and the transport is through the electronic band, the conductance reaches the plateau $\mathcal{G} = 2e^2/h$. We show that the 2/3-plateau evolves continuously with an increasing source-drain voltage to a 0.8-plateau or to a 0.4-plateau, depending on the gate voltage.
We also consider a system of a double quantum dot (2QD) and the influence of electron correlations on transport. The electron correlations within the 2QD were treated exactly, whereas the coupling of the 2QD to the leads was considered within an approximation which is valid for temperatures above the Kondo limit. We analyse the evolution of the gate voltage dependence of the spin correlation functions and the conductance with the change of the inter- and intra-dot repulsion. For weak to moderate correlations the physics of the device is dominated by the ground state eigenstates of the 2QD and antiferromagnetic correlations in the case of the double occupied 2QD. With increase of the on-site Coulomb repulsion above some threshold we observe a significant reduction of the antiferromagnetic coupling between the dots together with enhanced occupation of the triplet states. The current-voltage $(I - V)$ characteristics of the device exhibits multiple steps which are related to activation of the excited eigenstates of the 2QD, which are not normally seen in the gate voltage dependence for the zero bias. We also analyse the asymmetry of the $I - V$ characteristics of the device for the case of inequivalent couplings to the leads and find that a diode-type behaviour of the system can be linked to changed ratio of the occupation of the singlet and triplet 2QD eigenstates with the change of polarity of the device.

10 The interplay between superconductivity and magnetism

Herbert Capellmann

Inst Theor Physics, RWTH-Aachen, 52074 Aachen, Germany

capell@physik.rwth-aachen.de

The traditional concepts of the mutual influence of magnetism and superconductivity (singlet and triplet) are reviewed. The advent of heavy fermion superconductivity and in particular high T_c superconductivity and more recent claims of possible coexistence of itinerant magnetism and superconductivity led to drastic changes of these concepts. Experimental results about magnetic fluctuations will be confronted with the new and old ideas.

11 Fröhlich polarons from 0D to 3D: concepts and recent developments

Jozef Devreese

TFVS, Departement Fysica, Universiteit Antwerpen, Universiteitsplein 1, 2610 Antwerpen, Belgium

`Jozef.Devreese@ua.ac.be`

I analyse our present understanding of the Fröhlich polaron with emphasis on the response properties, in particular optical absorption. The structure of the presentation is as follows:

1. The Fröhlich polaron concept
   - All-coupling theory: The Feynman path integral. Comparison with the Monte Carlo schemes
   - Scaling relations for polarons in 2D and in 3D
2. Polaron response in 3D
   - Polaron mobility
   - Optical absorption of a polaron at arbitrary coupling
   - Polaron cyclotron resonance
3. Many-polaron systems in 3D and in 2D
   - Path-integral approach to the many-polaron problem
   - Optical absorption of many-polaron systems
   - Ripplopolarons in multi-electron bubbles in liquid helium
4. Polarons in 2D and in quasi-2D structures
   - Polarons in quantum wells
   - Cyclotron resonance in a quasi-2D many-polaron system and the role of screening
5. Polarons in quasi-0D structures
   - Many-polaron systems in quantum dots
   - Non-adiabaticity of polaronic excitons in semiconductor quantum dots. Photoluminescence and Raman scattering of polarons in quantum dots

12 Liquid-liquid phase separation in metal-ammonia solutions: was Ogg or Mott right?

Peter Edwards

Inorganic Chemistry Laboratory, University of Oxford, South Parks Road, Oxford OX1 3QR, UK

peter.edwards@chem.ox.ac.uk

Fluid solutions of alkali metals in anhydrous liquid ammonia are one of the most venerable areas of chemistry with a history dating back to the unpublished work of Sir Humphry Davy almost two centuries ago. Such 'metal-solutions' were much-beloved by Sir Nevill, who was particularly interested in the bewildering array of species existing in solution (e. g., solvated electrons,bipolarons), the composition-induced (intense blue) electrolyte-to-(copper-gold) liquid metal electronic transition, and the remarkable liquid-liquid phase separation. From extensive studies of metal solutions, Richard Ogg in 1946 first proposed the fascinating notion of Bose Einstein Condensation of trapped electron pairs; Ogg was also responsible for the first-ever report of high-temperature superconductivity, and that for vitreous, quenched sodium-ammonia solutions. In this presentation we review the nature of such interrelated issues in metal-ammonia solutions as a tribute to... Mott's Physics — and Ogg's Chemistry ... or is it the other way around?

13 Non-Fermi liquid behaviour of a Fermi gas with a repulsion

Konstantin Efetov and I L Aleiner

Department of Physics, Ruhr Universität Bochum, Universitätstraße 150, 44801 Bochum, Germany

efetov@tp3.rub.de

We suggest a new method of calculations for a clean Fermi gas with a repulsion in any dimension. This method is based on writing equations for quasiclassical Green functions and reducing them to equations for collective spin and charge excitations. The spin excitations interact with each other and this leads to non-trivial physics. Writing the solution of the equations and the partition function in terms of a functional integral over supervectors and averaging over fluctuating fields we come to an effective field theory describing the spin excitations. In some respects, the theory is similar to bosonization but also includes the "ghost" excitations which prevents overcounting of the degrees of freedom. Expansion in the interaction reveals logarithmic in temperature corrections. This enables us to suggest a renormalization group scheme and derive renormalization group equations. Solving these equations and using their solutions for calculating thermodynamic quantities we obtain explicit expression for the specific heat containing only an effective amplitude of the backward scattering. This amplitude has a complicated dependence on the logarithm of temperature, which leads to a non-trivial temperature dependence of the specific heat.

14 Luttinger liquid, Peierls or Mott insulator: Quantum phase transitions in one-dimensional electron-phonon systems

Holger Fehske

Institut für Physik, Universität Greifswald, Domstraße 10 a, D-17489 Greifswald, Germany

holger.fehske@physik.uni-greifswald.de

The challenge of understanding metal-insulator and insulator-insulator quantum phase transitions in 1D has stimulated intense work on generic microscopic models of interacting electrons and phonons. Combining Lanczos diagonalization with Chebyshev moment expansion and density matrix renormalisation group techniques we present unbiased results for ground-state and spectral properties of the Holstein Hubbard model at half-filling. For the spinless fermion case, we identify four distinct regimes of the phase diagram, corresponding to an attractive or repulsive Luttinger liquid at weak electron-phonon (EP) coupling, and an band-insulator or polaronic superlattice at strong coupling. Electron and phonon spectra reveal substantially different physics in these regimes and beyond indicate that the size of the phonon frequency significantly affects the nature of the Peierls transition. For the spinful case, with respect to the metal the electron-electron interaction favours a Mott insulating state, whereas the EP interaction tends to establish a Peierls state with true CDW long-range order. While polaronic features emerge only at strong EP couplings, pronounced phonon signatures, such as multi-quanta bound states, can be found in the Mott insulating regime as well. In order to corroborate the Mott to Peierls transition scenario, we determine the spin and charge excitation gaps and comment on the spin-charge separation phenomenon.

15 Spin-charge separation phenomena in quantum nanowires: theory and experiment

Yurii Firsov

Solid State Physics Division, Ioffe Institute, 26 Polytekhnicheskaya, 194021 St Petersburg, Russia

yuaf@icomefrom.ru

Electron-electron (e-e) correlations play the dominant role in one dimension (1D). As a result, the physical properties of a 1D metal are expected to be dramatically different from those of the usual Fermi liquid. In the absence of long-range interactions, a 1D electron liquid, the so-called Luttinger liquid (LL), is formed (while with long-range Coulomb interaction we have a 1D Wigner "crystal"). The most significant consequence is the absence of quasiparticle excitations in LL: instead, collective excitations associated with separate spin and charge degrees of freedom, moving with different velocities, are developed (the spin-charge separation phenomenon). The energy density of states around the Fermi energy decreases to zero (pseudogap), resulting in a power-law zero-bias anomaly for conduction if impurities in 1D or nanoconstrictions (weak links) in nanowires act as tunnelling contacts leading to nonlinear $I-V$ curves, with exponents depending on the strength of e-e interaction. An external magnetic field H affects the spin degrees of freedom (due to the Zeeman term in the initial Hamiltonian) and destroys spin-charge separation, making exponents of $I-V$ curves dependent on H, which leads to unconventionally strong magnetoresistance: for $H = 10$ tesla magnetoconductance may decrease by a factor of 10 or more). Investigation of the influence of spin-charge separation on thermal conductance in quantum nanowires shows that heat transfer is carried out by spinons (collective spin excitations); meanwhile, electric current is due to "holons" — collective charge waves. Inasmuch as charge and heat transport are realized by different types of collective excitations and the mechanism of heat transport is diffusion but electric current is carried out by holons tunnelling through weak links, the Wiedemann-Franz law may be strongly violated. Different realizations of 1D and quasi-1D systems (isolated quantum nanowires, carbon nanotubes and a quasi-1D system of ultrathin InSb nanowires periodically packed in an asbestos matrix) will be discussed and the theoretical predictions mentioned above will be compared with the experimental data.

16 Is there ballistic transport in metallic nanoobjects? Ballistic versus diffusive transport

Nicolás García, A P Levanyuk, Bai Ming and Lu Yonghua

LFSPyN, CSIC, Serrano 144, 28006 Madrid, Spain

nicolas.garcia@fsp.csic.es

We have studied the concept of ballistic resistance taking into account the classical Boltzmann contribution of metallic rough surfaces, that is to say the nonspecular resistance of the walls delimiting the objects where the current flows. It is seen and known that in metallic nanoobjects the mean free path of the electrons is largely reduced due to nonspecular scattering. It is so reduced that the mean free path is given by the smaller transversal size of the object. In the case of objects smaller than the mean free path of the electrons in the bulk material all electron transport properties are controlled by the size of the object. This establishes serious difficulties to obtain ballisticity since this requires that the mean free path is larger than the object's size. Our findings are applied to calculate the serial resistance in metallic nanoconstrictions and found that these are of the order of the quantum values of resistance. We will present experiments on transport in thin film constrictions and ballistic transport is not observed.

17 Carrier-density effects in many-polaron systems

Martin Hohenadler, J Loos and H Fehske

Institute for Theoretical and Computational Physics, TU Graz, Petersgasse 16, 8010 Graz, Austria

hohenadl@itp.tu-graz.ac.at

Many-polaron systems with finite charge-carrier density are often realized experimentally. Whereas density effects have been neglected in previous work on models with one electron or assuming independent carriers, here interaction effects arising from the overlap of individual polarons are addressed. Numerical and analytical methods are employed to calculate mainly photoemission spectra in the framework of the one-dimensional spinless Holstein model to reveal the nature of the quasiparticles in the system. For parameters favouring quasifree electrons or small polarons, no significant dependence on carrier density is observed. However, in the realistic adiabatic, intermediate-coupling regime, a cross-over from a polaronic system at low density to a rather metallic system at high densities is observed which may also play a role in some novel materials.

18 Magnetic quantum oscillations in nanowires

Viktor Kabanov and A S Alexandrov

Complex matter, Jožef Stefan Institute, Jamova 39, Ljubljana 1000, Slovenia

viktor.kabanov@ijs.si

Analytical expressions for the magnetization and the longitudinal conductivity of nanowires are derived in a magnetic field, B. We show that the interplay between size and magnetic field energy-level quantizations manifests itself through novel magnetic quantum oscillations in metallic nanowires. There are three characteristic frequencies of de Haas-van Alphen (dHvA) and Shubnikov-de Haas (SdH) oscillations, $F = F_0/(1+\gamma)^{3/2}$, and $F^{\pm} = 2F_0/|1+\gamma \pm (1+\gamma)^{1/2}|$, in contrast with a single frequency $F_0 = S_F/(2\pi e\hbar)$ in simple bulk metals. The amplitude of oscillations is strongly enhanced in some "magic" magnetic fields. The wire cross-section S can be measured using the oscillations as $S = 4\pi^2 S_F/(\gamma e^2 B^2)$ along with the Fermi surface cross-section, S_F.

19 Monte Carlo simulations of lattice polarons and bipolarons

Pavel Kornilovitch

Hewlett-Packard Company, Mail Stop 321A, 1000 NE Circle Blvd, Corvallis, Oregon 97330, USA

pavel.kornilovich@hp.com

Analytical integration of ionic degrees of freedom greatly simplifies the polaron problem by reducing it to one self-interacting particle. Such a system can be efficiently simulated by path-integral Quantum Monte Carlo methods on infinite lattices of any symmetry. In the last decade this idea has been extended to the calculation of polaron mass, spectrum, and density of states. In addition, the systematic error introduced by finite time steps has been eliminated through reformulation in continuous imaginary time. Those advances resulted in a powerful and versatile computational method capable of analyzing complex electron-phonon models, in particular models with long-range interactions. This brings us closer to the ability to simulate non-adiabatic effects in real materials from first principles. In this talk I review some old results obtained with this method as well as the newest developments, which include the extension to two-polaron (bipolaron) systems, singlet-triplet splitting, and dispersive phonons.

20 Condensation of Exciton Polaritons

Peter Littlewood[1], F M Marchetti[1], J. Keeling[2], M. H. Szymanska[3]

[1]*Cavendish Laboratory, University of Cambridge, JJ Thomson Ave, Cambridge CB3 0HE, UK*
[2]*Department of Physics, MIT, Cambridge, MA 02138, USA*
[3]*Department of Physics, University of Oxford, Oxford, UK*

pbl21@cam.ac.uk

By shining light on a semiconductor, one creates pairs of electrons and holes that bind together with the Coulomb interaction to make a neutral "atom" called an exciton — the solid state analog of positronium. The possibility that a gas of excitons might undergo Bose-Einstein condensation was raised over 40 years ago, but despite considerable effort and many beautiful experiments, no unequivocal observation has been made.

I will discuss some recent experiments with optical microcavities that make use of the mixing of excitons with photons into a bosonic particle called a polariton. In semiconductor microcavities, the polariton mass may be as light as 10^{-5} m_e, degeneracy temperatures of tens of degrees Kelvin can be readily reached, and recent experiments have shown strong evidence for a coherent ground state evolving out of a thermalised distribution of quasiparticles. However, the systems are open — polaritons decay — and so the existence of a true condensate is then a delicate balance between the many-body interactions favouring condensation, and the decoherence induced by pumping. And since the characteristic of the condensate is phase coherence, one must make a distinction — if one can — between BEC of polaritons and a more conventional laser.

I will argue that much of the physics is captured by a model system of two-level oscillators coupled to photons, and to external baths allowing for pumping and decay. (A similar model has also been used to describe superconductivity in ultracold atomic fermi gases, mediated by a quasi-molecular Feshbach resonance.) The solution of this model (phase diagram,and excitation spectra) help to clarify some central conceptual points, and can be compared directly to experiments.

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21 Non-Fermi liquid behaviour and pseudogap opening in the 2D Hubbard model within COM

Ferdinando Mancini and Adolfo Avella

Dipartimento di Fisica "E.R. Caianiello", Università degli Studi di Salerno, Via S Allende, 84081 Baronissi (SA), Italy

mancini@sa.infn.it

The two-dimensional Hubbard model is studied within the Composite Operator Method (COM) with the electronic self-energy computed in the Self-Consistent Born Approximation (SCBA). The main idea of the COM is to describe interacting electrons in terms of the composite elementary excitations appearing in the system owing to the strong correlations; the residual interactions among these excitations are treated within the SCBA. By analyzing the spectral function $A(\mathbf{k}, \omega)$, the momentum distribution function $n(\mathbf{k})$ and the Fermi surface on varying the filling, we find, at high doping, the ordinary Fermi-liquid behaviour of a weakly-interacting metal and, at low doping, anomalous features, signaling a non-Fermi-liquid behaviour, and the opening of a pseudogap, as reported for cuprate superconductors.

22 Functional properties of molecular $MoSI_x$ nanowires: from structure to magnetism

Dragan Mihailović

Complex Matter, Jožef Stefan Institute, Jamova 39, 1000 Ljubljana, Slovenia

dragan.mihailovic@ijs.si

Inorganic molecular nanowires with the general formula $Mo_xS_yI_z$ have been shown to exhibit a variety of basic functional properties in which they display performance which is superior to other one-dimensional nanomaterials. Because of their purity, ease of synthesis and ease of dispersion they have already been heralded as a serious alternative to carbon nanotubes for quite a few applications. In this presentation we will give an overview of the basic properties of $MoSI_x$ nanowires, ranging from synthesis, fundamental physical and chemical properties to emerging applications in nanoelectronics and biomedical nanodevices. The structure of the individual $MoSI_x$ nanowires is shown to be best described in terms of a one-dimensional polymer composed of a string of rigid Mo-chalcogenide-halide clusters joined together by S bridges. While their longitudinal Young's modulus is very high, these 1D chains are exceptionally weakly bound together into bundles, leading to easy dispersion in a variety of solvents. Unlike carbon nanotubes, the nanowires can be dispersed and functionalised in water and other polar solvents. The stability of individual wires in air and in solution is confirmed by AFM measurements. The weak lateral bonds between nanowires lead to low sliding friction. This makes them of great potential interest for tribological applications and — in combination with the exceptional dispersion characteristics — useful components of self-lubricating composites. The functional properties relevant for nanoscale device fabrication will be discussed in more detail, particularly dispersion characteristics, functionalisation and attachment to gold particles and self-assembly upon synthesis. DFT calculations show that $MoSI_x$ nanowires are expected to be either metallic, semimetallic or semiconducting, depending on their stoichiometry. The basic stoichiometric compound $Mo_6S_3I_6$ is calculated to have narrow electronic bands crossing the Fermi energy, with a large density of states at E_F. Transport measurements on moly-paper, pressed pellets and single bundles all reveal similar variable-range-hopping behaviour, suggesting localisation of carriers occurs on undoped NWs. Calculations also suggest remarkable non-linear mechanical, electronic and magnetic properties arising from the bistability of the S bridges.

23 Disorder and interaction effects in one dimension

Michael Pepper, A C Graham and K J Thomas

Cavendish Laboratory, University of Cambridge, J J Thomson Avenue, Cambridge CB3 0HE, UK

mp10000@cam.ac.uk

The technology of producing electrons confined so that the momentum is only free to change in one dimension is now of sufficient quality that 20 one-dimensional 1D subbands can be observed via the plateaux of quantised conductance. Such effects can be explained on the basis of straightforward one-electron considerations; however plateaux, or structure, appearing at non-quantised values appear to arise from the interaction between the electrons.The best known of these effects is the 0.7 structure which has been widely observed in a range of 1D nanodevices; there are various theories of this phenomenon which will be reviewed in the light of experimental results strongly suggesting that electron spin plays a crucial role. It will be shown that the 0.7 is the first of a series of instabilities which occur whenever spin up and spin down levels cross, these additional non-quantised plateaux are termed 0.7 analogues in view of the strong similarities between their behaviour and that of the 0.7. The role of disorder in the observation of these effects will be discussed.

24 Fabrication and electronic properties of perfect quantum wires and dots with subnanometre dimensions

Klaus Ploog, S Fölsch, J Lagoute

Paul Drude Institute for Solid State Electronics, Hausvogteiplatz 5-7, 10117 Berlin, Germany

ploog@pdi-berlin.de

We have used low-temperature scanning tunnelling microscopy (LT-STM) and spectroscopy (LT-STS) to assemble surface-supported Cu quantum wires and Cu adatom islands of successive size atom-by atom at 7 K on Cu(111) surfaces and to study their distinct electronic properties. These ultrathin metallic chains represent an ideal 1D electronic model system which may serve as nanowires for the interconnection of molecular building blocks in molecular electronics. Our LT-STS experiments have revealed a series of electronic eigenstates that are localized in the Cu chains. Spatially resolved maps of the local density of states evidence a 1D quantum confinement that is perfectly described by an effective 1D tight-binding Hamiltonian [1]. In order to study the effect of kinks and branches in these nanowires, V- and Y-shaped chains of Cu atoms on Cu(111) were fabricated by atom-by-atom manipulation. It is important to note that the junction is stabilized by a compact Cu trimer, while the extremities for V and Y consist of close-packed monatomic Cu chains along the in-plane $< 110 >$ directions [2]. As the wave function confinement of both straight atomic chains as well as branched structures of artificial nanowires can be described by a linear combination of atomic orbitals (LCAO), which is a rather simple approach, the description of more complex quantum-wire structures and the prediction of their electronic properties becomes feasible.

Finally, we have fabricated native Cu adatom islands "dots" consisting of only a few atoms to explore how electronic properties evolve with size. Starting from the single Cu adatom, we observe the formation of a series of quantum states, which merge into the traditional Shockley surface state in the limit of large islands. Our results evidence a natural link between this archetypal surface property, the quantum confinement in compact adatom structures, and the sp hybrid state associated with the discrete atom [3]. This is an important step forward to tailor magnetic and electronic surface properties by controlling size, geometry and composition at the atomic level.

References

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25 The Single-Atom Transistor: An approach towards quantum electronics at room temperature

Thomas Schimmel

Institut für Angewandte Physik, Universität Karlsruhe, 76128 Karlsruhe, Germany

thomas.schimmel@physik.uni-karlsruhe.de

Using a novel electrochemical approach, we demonstrate the fabrication of bistable atomic-scale metallic point contacts, which can be reproducibly opened and closed by means of a voltage applied to an independent third electrode used as a gate electrode [1]. In this way, an electrical circuit can be opened and closed by the controlled and reproducible reconfiguration of the contacting atoms. After the fabrication of the atomic-scale contact by electrochemical deposition of silver within a nanoscale gap, the bistable configuration of the contact is achieved by an electrochemical cycling process. When the contact is closed, is shows conductance quantization, the conductance being $G_0 = 2e^2/h$ or predefined multiples of this value, the on-state conductance being controlled by the cycling parameters. The device reproducibly operates at room temperature. It represents a first demonstration of an atomic relay or transistor, opening intriguing perspectives for the emerging fields of quantum electronics and logics on the atomic scale.

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26 A glimpse into subnano structures

Arndt Simon

Max-Planck-Institut für Festkörperforschung, Heisenbergstraße 1, 70569 Stuttgart, Germany

A.Simon@fkf.mpg.de

"Macro-", "micro-", "nano-"...what will come next? Modest "subnano" or more challenging "pico"? The bottom-up route into subnano structures is well established. It lies at the heart of chemistry.
Metal cluster compounds provide a versatile subnano scale construction kit. The clusters consist of a core of metal atoms surrounded by non-metal atoms, and their arrangement in a solid results quasi in a dispersion of little pieces of metal in a dielectric matrix. Low dimensionality is easily achieved ranging from zero- to three-dimensional interconnections. Metal clusters often accumulate non-metal atoms inside and can then be condensed into dispersions of subnano pieces of salt in a metallic matrix. These structures relate to quantum dot and antiquantum dot arrays, however, two orders of magnitude smaller than those produced by artificial structuring along a top-down route. Some properties of such self-assembled structures will be discussed.

27 Localisation vs. delocalisation in correlated nanosystems within exact diagonalisation — ab initio approach

Józef Spałek

Institute of Physics, Jagiellonian University, Reymonta 4, 30-059 Kraków, Poland

ufspalek@if.uj.edu.pl

The question how small a piece of (quantum) wire can be, is of fundamental nature. To address this question, we have used the exact diagonalisation of the system up to 16 atomic sites combined with ab initio readjustment of single-particle wave functions in the resultant (correlated) state (EDABI method). In this manner, the properties of the nanowires have been calculated as a function of interatomic distance. The evolution of the Fermi-Dirac-like distribution, as well as the Luttinger liquid effects, are discussed for these nanosystems. A comparison with the exact Lieb-Wu solution for an infinite chain is made.
The role of boundary condition is highly nontrivial.
In the second part, we discuss the tunneling conductivity through simple one- and two-site systems within the same method. A comparison with quantum dots exhibiting the Kondo effect is made.

28 Trapping and Self-Trapping: Polaronic Defects in the bulk and at interfaces

Marshall Stoneham

Physics and Astronomy, University College London, Gower St, London WC1E 6BT, UK

ucapams@ucl.ac.uk

Polarons are commonly discussed using as a framework the analytical theories of Fröhlich or of Holstein, sometimes including Landau's recognition of a barrier to self-trapping. Yet these pictures give a very limited, sometimes misleading, description of real systems. Qualitative inconsistencies can arise when ionic and electronic polarisations are merged too casually, or when coupling is assumed to be to just one mode, often taken as longitudinal optic phonons. Electron, hole, and excitonic polarons have their own special features. Generalisations are needed when there are other degrees of freedom, whether spin, or Jahn-Teller interactions, or when an electronic excitation is involved. I shall discuss some representative cases for which theory and experiment can be compared in detail. Experimental data for surfaces and interfaces are limited, although key extra features can be identified, like space charge, altered Madelung terms, reconstructions, and effects associated with asymmetry across the interface, including image interactions, the Rashba effect, and altered selection rules.

29 Organic semiconductors for spintronics

Carlo Taliani

ISMN-Bologna, CNR, Via P Gobetti 101, 40129 Bologna, Italy

C.Taliani@ism.bo.cnr.it

There has been an increasing effort in recent years to develop a new electronics based on the manipulation of the spins rather than charges. The development of Spintronics requires semiconductors able to transport spin without significant losses at room temperature. This is particularly difficult in the case of ordinary semiconductors because of the conductivity mismatch between semiconductors and spin-injecting electrodes.

Based on our background experience in the area of organic semiconductors since the development of the organic based FET (1) and Organic Light Emitting Diode (OLED) (2), we have explored for the first time the potential of organic semiconductors for the practical development of spintronics for the extremely low spin scattering rate compared to ordinary inorganic semiconductors.

We fabricate CMR manganites electrodes by the innovative method of Pulsed Plasma Deposition. $La_{0.7}Sr_{0.3}MnO_3$ (LSMO) thin films have 100% spin polarization at RT. The prototypical organic semiconductor sexithienyl (T_6), is deposited by UHV deposition on a nanostructured channel (80-500 nm) of the planar LSMO/T_6/ LSMO device acting efficiently as a spin-valve *at room temperature* (3). The spin transfer coherence length is estimated to be about 200–300 nm indicating a spin scattering time T_1 of the order of 10^{-6} s.

This experiment has given the first evidence of spin coherent injection and transfer in organic semiconductors and has opened the field of Organic Spintronics.

Spin polarized electrodes have been also applied to OLED configurations showing efficient hole injection in a TPD/AlQ_3 OLED structure (4) with a 6 V turns on voltage.

The invention of spin injection at the CMR/organic semiconductor interface opens the way to application in organic electronics and optoelectronics. The hybrid spin-valve offers the possibility to generate dense low energy consumption memory elements and magnetic sensors, and the applications in optoelectronics may allow to generate new interesting physics and devices based on the multi-functionality of CMR/organic interface by controlling the recombination spin statistics of carriers. Recent results on the development of conventional and novel FM top electrode OLED structures will be presented.

Preliminary results concerning the ns time-resolved electroluminescent spectroscopy applied to conventional and spin polarized light emitting devices will be presented as well.

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30 Magnetic polarons and phase separation in the Kondo model

Wolfgang von der Linden

Institute of Theoretical and Computational Physics, Graz University of Technology, Petersgasse 16, 8010 Graz, Austria

wvl@itp.tu-graz.ac.at

The ferromagnetic Kondo model with classical corespins is studied by unbiased Monte-Carlo simulations. We show that with realistic parameters for the manganites and at low temperatures, the double-exchange mechanism does not lead to phase separation but rather stabilizes individual ferromagnetic polarons. Within the ferromagnetic polaron picture, the pseudogap in the one-particle spectral function $A_k(\omega)$ can easily be explained. We present a simplified physical model, which can easily be evaluated numerically and provides a simple qualitative understanding of the physical features of the ferromagnetic Kondo model.