

# Highly correlated systems and general field theory applications

## 5 - 1 – The Kondo necklace model with planar anisotropy

Mendoza-Arenas, J.J.,<sup>1</sup> Franco, R.,<sup>1</sup> and Silva-Valencia, J.<sup>1</sup>

<sup>1</sup>*Departamento de Física, Universidad Nacional de Colombia, Bogotá*

Heavy fermion systems generate great interest in condensed matter physics due to the diverse properties they present at low temperatures. Materials of this kind, like metallic compounds containing rare-earth or actinide elements as Yb, Ce and U, possess two types of electrons: the conduction electrons in the  $s$ ,  $p$  and  $d$  orbitals, and the localized ones, which stay in the  $f$  orbitals. The interaction of this electrons leads to two different effects, which compete between them to determine the magnetic behavior of the system. The first, known as the Kondo effect, is the screening of the localized magnetic moments due to the conduction electrons, which produces singlets along the system. The second, called RKKY interaction, is an indirect exchange between the spins of the localized electrons, mediated by the conduction ones, and tries to establish an antiferromagnetic order.

One of the models used to study the competition between these effects and focus on the resulting magnetic behavior (non magnetic spin liquid or antiferromagnetic phase) is the Kondo necklace. In this model, the charge degrees of freedom are completely neglected, and only spin degrees are kept. In order to achieve this, the conduction electrons are replaced by a  $1/2$  spin chain with  $XY$  interaction. In the Hamiltonian, the interaction between the localized and conduction spins is characterized by the parameter  $J$ , and the  $XY$  interaction in the conduction chain by the parameter  $t$ .

The analysis of this model by different methods such as quantum Monte Carlo, bosonization and density matrix renormalization group (DMRG) has established that, in one dimension, any finite value of  $J/t$  gives a spin liquid phase (critical point  $(J/t)_c = 0$ ). Nevertheless, the inclusion of an anisotropy  $\eta$  in the  $XY$  interaction of the conduction chain can cause a phase transition to an antiferromagnetic ordering. In the present work we investigate the consequences of this anisotropy in the phase diagram of the model using DMRG, so that we can treat large systems with high precision. First, we study the ground state energy. Then, we calculate the energy gap between the states having total spin 0 (singlet) and 1 (triplet), from  $\eta = 0$  (original Kondo necklace model) to  $\eta = 1$  (fully anisotropic model). The critical points are those in which the gap is 0. We obtain that for any  $\eta \neq 0$  a finite value of  $(J/t)_c$  exists. With these results we construct the phase diagram of the model.

## 5 - 2 – Spatial range of the Kondo effect

Büsser, C.A.,<sup>1</sup> Martins, G.B.,<sup>1</sup> Costa Ribeiro, L.,<sup>2</sup> Dagotto, E.,<sup>3</sup> and Anda, E.V.<sup>2</sup>

<sup>1</sup>*Department of Physics, Oakland University, Rochester, MI, USA.*

<sup>2</sup>*Departamento de física da Pontificia Universidade Católica do Rio de Janeiro, Brazil.*

<sup>3</sup>*CMSD - Oak Ridge National Laboratory, Oak Ridge, TN and University of Tennessee, Knoxville TN, USA.*

The objective of this work is to discuss the spatial range of the effect caused by the Coulomb interaction localized at an impurity center.

The numerical method we use, the embedded cluster approximation (ECA) and the finite U slave bosons mean fields (FU-SBMF), are developed to treat localized impurity systems that consist in general of a central many-body interacting region weakly coupled to a one-body non-interacting conduction band. It is important to note that, contrary to the Numerical Renormalization Group technique, ECA and FUSB can work in real space.

Within this work, a comparison between ECA and the FU-SBMF will be presented. Using these two techniques, we will discuss the spatial length of the Kondo screening cloud, which can be estimated as  $R_K \approx \hbar v_F / k_B T_K$ , where  $v_F$  is the bulk Fermi velocity and  $T_K$  is the Kondo temperature[1]. While this expression gives the correct scale for  $R_K$  it will fail to give the exact value as the quasi-particles will not propagate with  $v_F$ . We will check, within ECA and FU-SBMF, the validity of this relationship and a correct value for the propagation of the quasi-particles will be introduced.

Instead of using the spin-spin correlation to determine the length of the Kondo cloud, we will use the local density of states (LDOS) on the metal host, far from the impurity. The presence of the impurity produce a disturbance in the LDOS of sites away from it. In this work, we propose a way of using this distortion to evaluate the spatial range of the Kondo effect. We observe that the effect of the distortion decays exponentially as a function of the distance from the impurity. In view of that, a characteristic length  $\hat{R}_K$  can be easily defined. When the coupling between the impurity and the metal is increased, we verify that  $\hat{R}_K \sim 1/T_K$ . In addition, the real propagation velocity for the quasi-particles can be estimated.

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### 5 - 3 – Unexpected charge effects in Mott insulators: Magnetoelectric behavior of Cr-trimer complexes

Ayala Valenzuela, O.,<sup>1,2</sup> McDonald, R.D.,<sup>1</sup> Jaime, M.,<sup>1</sup> and Mydosh, J.A.<sup>3</sup>

<sup>1</sup>*National High Magnetic Field Laboratory, Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA*

<sup>2</sup>*Centro de Investigación en Materiales Avanzados S. C., Miguel de Cervantes 120, Complejo Ind. Chihuahua, Chihuahua 31120, México*

<sup>3</sup>*Institute of Physics II, University of Cologne, 50937 Cologne, Germany*

Mott insulators are of growing interest in condensed matter physics research largely because of the novel properties that arise upon tuning electron concentration away from half band filling. Among these very important materials are high-TC cuprate superconductors and colossal magnetoresistive manganites. Mott insulators are characterized by strong electron correlations, i.e. a large onsite Coulomb repulsion relative to the dominant electron hopping, localizing one electron per site at half-band filling. As a result the properties of these materials are commonly described solely in terms of their magnetic exchange interactions, for example quantum magnet systems.

Certain classes of Mott insulator have recently been predicted to break this paradigm. For a finite Coulomb interaction-electron hopping ratio, the kinetic energy gain due to the overlap with neighboring sites of opposite spin orientation allows for the possibility of real currents resulting from hopping around a closed loop. This provides a direct correlation between the magnetic spin texture and the dielectric properties of a material. The simplest loop is an isolated triangle such as the Cr-trimer systems investigated.

In this work we present measurements of the dielectric response as a function of magnetic field of Cr-trimer systems, which combined with recent theoretical developments indicates a multiferroic behavior evidenced by a purely electronic mechanism. Magnetic field strengths of the order of the exchange interaction ( $J \sim t^2/U$ ) strongly perturb the spin texture, which is evident as steps and plateaus in the magnetization behavior. The corresponding shifts in dielectric properties reveal the role of the charge degrees of freedom. Electron Spin Resonance (ESR) results and the prospect of novel dipole-active ESR giving rise to the possibility of negative refractive indices under special conditions, which will also be discussed.

### 5 - 4 – Entanglement and phase separation in a Bose mixture

Silva-Valencia, J.,<sup>1</sup> Franco, R.,<sup>1</sup> and Figueira, M.S.<sup>2</sup>

<sup>1</sup>*Departamento de Física, Universidad Nacional de Colombia, A. A. 5997, Bogotá, Colombia*

<sup>2</sup>*Instituto de Física, Universidade Federal Fluminense (UFF). Avenida litorânea s/n, CEP: 24210-346, Niterói, Rio de Janeiro, Brazil*

The physical properties of cold atoms trapped in optical lattices has been intensively studied in the last years, ever since the Bose-Einstein condensation of alkali atoms was observed[1]. After that, the development in trapping and cooling techniques lead to the realization of truly one-dimensional systems[2], as well as the manipulation of atom-atom interactions by Feshbach resonances, providing the opportunity to study many-body effects therein. Several interesting phenomena including the superfluid to Mott insulator transition have been observed in a one-dimensional optical lattices[3]. In the past years, many investigations have been carried out using a single species of bosonic atoms in optical lattices [4]. Recently cold bosonic mixtures, fermions and Bose-Fermi mixtures in optical lattices have attracted much attention [5,6]. Mixtures of different species are very interesting since additional phases could appear due to the interspecies interactions[7,8]. In this work, we study two species of bosonic atoms or equivalently, bosonic atoms with two relevant internal states using the density matrix renormalization group method [9] and the von Neumann entropy to measure the entanglement. Recently it had been shown that entanglement may be an effective indicator of quantum phase transition in spin and fermionic systems[10]. Here we calculate the one-site entropy as a function of inter and intra species interaction strengths and we identify different phases, such as: superfluid, Mott insulator and phase separation where different species reside in spatially separate regions. We found that the entanglement is able to signal quantum phase transitions between the superfluid phase, Mott insulator phase and phase separation state of the system.

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## 5 - 5 – Anderson impurity model: Double occupancy contribution to the magnetic susceptibility

Jaroszewicz, S.,<sup>1</sup> Roura-Bas, P.,<sup>1</sup> and Llois, A.M.<sup>1</sup>

<sup>1</sup>*Grupo Materia Condensada, Centro Atómico Constituyentes, C.N.E.A.*

After solving the single Anderson impurity model (SIAM) within the non crossing approximation with a finite Coulomb repulsion,  $U$ , and vertex corrections (NCAf2v), we focus on the magnetic susceptibility. Using the same diagrammatic expansion, the main contribution to the magnetic susceptibility comes from the singly occupied states and it can be dressed with two factors, namely, the double state occupancy and the vertex corrections. In this work we analyse the effect of double occupancy on the dynamic and static susceptibility as a function of  $U$  and of the degeneracy of the total impurity angular moment,  $J$ .

## 5 - 6 – Magnons versus deconfined spinons in finite quantum frustrated antiferromagnets

Hamad, I.J.,<sup>1</sup> Manuel, L.O.,<sup>1</sup> Feiguin, A.E.,<sup>2</sup> and Trumper, A.E.<sup>1</sup>

<sup>1</sup>*Instituto de Física Rosario (CONICET) and Universidad Nacional de Rosario, Bv. 27 de febrero 210 bis, (2000) Rosario, Argentina.*

<sup>2</sup>*Microsoft research, Station Q, University of California, Santa Barbara, California 93106, USA.*

We have investigated the confiability of using static and mobile vacancies to explore the possible realization of a fractionalization scenario in a finite frustrated Heisenberg model. Recently it has been hypothesized by Poilblanc *et al.* (Phys. Rev B **73** R100403 (2006)), that the reduction of the quasiparticle weights of doped static and mobile non magnetic impurities can be used to test the existence of a deconfined spinons in the doped  $J_1 - J_2 - J_3$  Heisenberg model. The good agreement we found between the self consistent Born approximation and exact diagonalization spectra indicates that the quasiparticle weight reduction in finite systems is due to the hole-magnon coupling instead of a spinon excitation liberated away from the hole. In the thermodynamic limit we found that for an ample range of the Brillouin zone the spectral functions are completely incoherent, thus leaving place for non conventional scenarios.

## 5 - 7 – Study of shot noise in normal - insulator - superconductor junction

Duque, M.F.<sup>1</sup> and Fonseca, F.R.<sup>1</sup>

<sup>1</sup>*Departamento de Física, Universidad Nacional de Colombia, Bogota, Colombia*

In this paper we calculate the shot noise differential and the current differential generated by the flow of charge carriers through a standard interface metal-insulator- superconductor. We calculate solutions of the Bogoliubov - De Gennes equations in the normal metal interfaces-insulator-superconductor, whereas the normal metal is at  $x < 0$ 's superconductor and the insulator is taken as a potential barrier width on the order of ( $nm$ ) that can be simulated by a Dirac delta function in which there may be tunnels. Transmission and Reflection coefficients of particles from the current flow are determined with the help of the solutions of Andreev reflection coefficients, electron-hole, and reflection electron-electron, which depend on the shot noise and current, finding the nature of the charge carriers using the fano factor. There is a dependence of shot noise and the current differential in regards to the potential difference between the normal metal and superconductor and the width of the insulating barrier, and how that behavior varies considering symmetry type parameter  $s$ ,  $d_{x^2-y^2}$  and  $d_x$ , of the superconductor.

## 5 - 8 – Shot noise and charge fluctuations in a double quantum dot chain

Díaz, S.A.<sup>1</sup> and Núñez, A.S.<sup>1</sup>

<sup>1</sup>*Departamento de Física, Facultad de Ciencias Físicas y Matemáticas, Universidad de Chile, Casilla 487-3, Código Postal 837-0415, Santiago, Chile*

We present the partial results of our theoretical investigations on the effect of electronic correlations on the structure of charge and current fluctuations on nanometric systems.

By coupling a finite Hubbard chain to electrodes, which then play the role of heat and electron reservoirs, we obtain a theoretical framework able to describe transport through a correlated electron system.

Following the non-equilibrium quantum mechanics technique described by Orellana and Claro [Phys. Rev. Lett. **90**, 178302 (2003)], we can impose an electric current running through it, and thereby study its effect on thermal and quantum fluctuations. We focus our study on the effects of electronic correlations on quantum fluctuations of the charge and spin currents.

Through the representation of the model in terms of integrals over quantum fields we are able to directly assess those fluctuations in terms of the customary non-equilibrium quantum field theory approach paved by the well known Keldysh formalism [Rammer and Smith. Rev. Mod. Phys. **58**, 323-359 (1986)]. This

approach has been successfully followed to study current driven spin fluctuations in metals and spin systems.

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## **5 - 9 – Anderson Impurity Model: Vertex corrections within the finite U Non-Crossing Approximation**

Roura-Bas, P.,<sup>1</sup> Vildosola, V.,<sup>1</sup> Manuel, L.O.,<sup>2</sup> and Llois, A.M.<sup>1</sup>

<sup>1</sup>*Grupo Materia Condensada, Centro Atómico Constituyentes, C.N.E.A.*

<sup>2</sup>*Instituto de Física Rosario, Universidad Nacional de Rosario, Rosario, Argentina*

We revise the simplest possible approximations to solve numerically the vertex equations for the Anderson Impurity Model within the finite U Non-Crossing Approximation (UNCA) considering the self energies at lowest order in  $1/N$ , that is, within the  $(1/N)^0$  diagrammatic expansion. We introduce an approximation to the vertex corrections that includes the double energy dependence and compare it with an approximation (NCAf2v) that neglects a second energy argument. Finally, we analyse the influence on the estimated Kondo scale for simple electronic models.

## **5 - 10 – Study of the tunneling current on an asymmetric Luttinger liquid with a Point contact.**

Fernandez, V.<sup>1</sup>

<sup>1</sup>*Depto de Física. UNLP IFLP. CONOCET. Argentina*

We study an asymmetric Luttinger Liquid with a point contact. We discuss the behavior of the tunneling current through the contact due to the difference on the velocities of the right and left movers.