

ISTITUTO NAZIONALE DI FISICA NUCLEARE

Preventivo per l'anno **2001**

Codice	Esperimento	Gruppo
	LF-11	4

Struttura
L.N.F.

Rappresentante Nazionale: C. NATOLI

Struttura di appartenenza: L.N.F.

Ricercatore responsabile locale: C. NATOLI

Posizione nell'I.N.F.N.: Dirigente di Ricerca

INFORMAZIONI GENERALI

Linea di ricerca	Elettroni fortemente correlati.
Laboratorio ove si raccolgono i dati	L.N.F.
Sigla dello esperimento assegnata dal Laboratorio	LF-11 Vedi Allegato n. 1
Acceleratore usato	
Fascio (sigla e caratteristiche)	
Processo fisico studiato	
Apparato strumentale utilizzato	
Sezioni partecipanti all'esperimento	LNF
Istituzioni esterne all'Ente partecipanti	
Durata esperimento	3 anni

Mod. EC. 1

(a cura del responsabile locale)

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PREVENTIVO LOCALE DI SPESA PER L'ANNO 2001

In ML

VOCI DI SPESA	DESCRIZIONE DELLA SPESA	IMPORTI		A cura della Comm.ne Scientifica Nazionale
		Parziali	Totale Compet.	
Viaggi e missioni	Interno			
	Inviti Ospiti Stranieri	10	10	
	Estero	12	12	
Materiale Consumo				
Trasp.e facch.				
Spese Calcolo	Consorzio			
	Ore CPU			
	Spazio Disco			
	Cassette			
	Altro			
Affitti e manutenz. apparecchiati.				
Materiale Inventariabile				
Costruzione Apparati				
Totale			22	
Note:				

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ALLEGATO MODELLO EC 2

Codice	Esperimento	Gruppo
	LF-11	4

Struttura
L.N.F.

PREVISIONE DI SPESA: PIANO FINANZIARIO LOCALE
PER GLI ANNI DELLA DURATA DEL PROGETTO

In ML

ANNI FINANZIARI	Miss. interno	Inviti Ospiti Stranieri	Miss. estero	Mater. di cons.	Trasp.e Facch.	Spese Calcolo	Affitti e manut. appar.	Mat. inventar.	Costruz. apparati	TOTALE Competenza
2001		10	12							22
2002		13	15							28
TOTALI		23	27							50

Note:

Osservazioni del Direttore della Struttura in merito alla disponibilità di personale e di attrezzature:

Mod. EC. 3

(a cura del responsabile locale)

ISTITUTO NAZIONALE DI FISICA NUCLEARE

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Codice	Esperimento	Gruppo
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Struttura
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PREVENTIVO GLOBALE PER L'ANNO 2001

In ML

Struttura	A CARICO DELL' I.N.F.N.										A carico di altri Enti
	Miss. interno	Ospiti Stran.	Miss. estero	Mater. di cons.	Trasp. e Facch.	Spese Calc.	Affitti e Manut. Appar.	Mater. inventar.	Costruz. appar.	TOTALE Compet.	
L.N.F.		10	12							22	0
TOTALI		10	12							22	0

NB. La colonna **A carico di altri Enti** deve essere compilata **obbligatoriamente**

Note:

Mod. EC. 4

(a cura del rappresentante nazionale)

ISTITUTO NAZIONALE DI FISICA NUCLEAREPreventivo per l'anno **2001**

Codice	Esperimento	Gruppo
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Struttura
L.N.F.

A) ATTIVITA' SVOLTA NELL'ANNO 2000

Applicazioni di metodi sviluppati per il modello di Hubbard alla descrizione realistica di materiali con ferro magnetismo a banda.

B) ATTIVITA' PREVISTA PER L'ANNO 2001

Descrizione di giunzioni metallo/semiconduttore nei nanotubi di fullerene.

C) FINANZIAMENTI GLOBALI AVUTI NEGLI ANNI PRECEDENTI

In ML

Anno Finanziario	Missioni interno	Ospiti Stran.	Missioni estero	Mater. di consumo	Trasp. e Facch.	Spese Calcolo	Affitti e Manut. Apparec.	Materiale inventar.	Costruz. apparati	TOTALE
2000		11	20							31
TOTALE		11	20							31

Mod. EC. 5

(a cura del rappresentante nazionale)

ISTITUTO NAZIONALE DI FISICA NUCLEAREPreventivo per l'anno **2001**

Codice	Esperimento	Gruppo
	LF-11	4

Struttura
L.N.F.

PREVISIONE DI SPESA**Piano finanziario globale di spesa****In ML**

ANNI FINANZIARI	Miss. interno	Inviti Ospiti Stranieri	Miss. estero	Mater. di cons.	Trasp.e Facch.	Spese Calcolo	Affitti e manut. appar.	Mat. inventar.	Costruz. apparati	TOTALE Competenza
2001		10	12							22
2002		13	15							28
TOTALI		23	27							50

Note:

Mod. EC. 6

(a cura del rappresentante nazionale)

Codice	Esperimento	Gruppo
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Struttura
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REFEREES DEL PROGETTO	
Cognome e Nome	Argomento
Anonimo Internazionale 1	
Anonimo Internazionale 2	

MILESTONES PROPOSTE PER IL 2001	
Data completamento	Descrizione

COMPETITIVITA' INTERNAZIONALE
I giudizi del referee 1: A (per originalità progetto e impatto potenziale), A (per raggiungibilità obiettivi in tempo), A (per competenza membri) I giudizi del referee 2: A, B, A

LEADERSHIPS NEL PROGETTO	
Cognome e Nome	Funzioni svolte

Codice	Esperimento	Gruppo
	LF-11	4

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Consuntivo anno 1999/2000

LAUREATI		
Cognome e Nome	Titolo della Tesi	Sbocco professionale
DANIELE Antonella Laurea in FISICA	Studio Strutturale di siti attivi in zinco proteine mediante la teoria di diffusione multipla con uso di potenziali complessi.	Università
Laurea in		
Laurea in		
Laurea in		
Laurea in		
DOTTORI di RICERCA		
CUOZZO Massimiliano Dott in FISICA	Correlazione elettronica, Ordine Orbitale e di in in V2O3 studiata tramite la diffrazione anomala risonante.	Industria
Dott in		
Dott in		
Dott in		
PRESENTAZIONI A CONFERENZE SU INVITO E SEMINARI SIGNIFICATIVI		
Relatore	Titolo	Conferenza o luogo

Codice	Esperimento	Gruppo
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Consuntivo anno 1999/2000

SIGNIFICATIVE VARIAZIONI DI BILANCIO

Capitolo	Variazione (ML)	Motivazione
Missioni Interne	_____	
Missioni Estere	_____	
Consumo	_____	
Trasporti e Facchinaggio	_____	
Spese Calcolo	_____	
Affitti e Manutenzioni	_____	
Materiale Inventariabile	_____	
Costruzione Apparati	_____	
Totale storni	_____	

CONFERENZE, WORKSHOP e SCUOLE ORGANIZZATE in ITALIA

Data	Titolo	Luogo
24-09-2000	Nanotubes and Nanostructures 2000	S. Margherita di Pula (CA)

SIGNIFICATIVE COMMESSE E RELATIVO IMPORTO

ANAGRAFICA FORNITORE	DESCRIZIONE PRODOTTO O COMMESSA	IMPORTO (ML)

Codice	Esperimento	Gruppo
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Consuntivo anno 1999/2000**MILESTONES RAGGIUNTE**

Data completamento	Descrizione
Commento al conseguimento delle milestones	

SVILUPPO DI STRUMENTAZIONE INNOVATIVA

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Ricadute su altri gruppi, sul sistema industriale e su altre discipline

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Elenco delle pubblicazioni anno 1999/2000

- [1] M. Benfatto, Y. Joly and C.R. Natoli, Critical reexamination of the experimental evidence of orbital ordering in LaMnO_3 and $\text{La}_{0.5}\text{Sr}_{1.5}\text{MnO}_4$. Phys. Rev. Lett. in press.
- [2] 1999 "On the Coulomb interaction in chiral-invariant one-dimensional electron system", S. Bellucci and J. Gonzalez, cond-mat/9903022, European Physical Journal B (submitted).
- [3] 1998 "Renormalization of the Coulomb interaction in one-dimensional electron systems", S. Bellucci and J. Gonzalez, cond-mat/9802011, Physical Review B (submitted), (3 citations).
- [4] 1999 "Long-range interactions in a one-dimensional electron system", S. Bellucci, Proceedings of the 6th Conference on Path Integrals, (Florence, 25-29 August 1998), edited by R. Casalbuoni, R. Giachetti, V. Tognetti, R. Vaia, P. Verrucchi, page 363, hep-th/9810181, (1citation).

Esperimento	Gruppo
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ALLEGATO 1**LF-11**

(Proposta 2001 - 2002)

Qui di seguito e' descritta l'Iniziativa Specifica LF11. Questa iniziativa si propone di ottenere risultati innovativi nel campo degli studi teorici e della fenomenologia della fisica della materia. Essa comprende attivita' che, utilizzando anche metodi numerici di indagine, potenziano le connessioni interdisciplinari tra la teoria dei campi e la meccanica statistica, con importanti ricadute anche nello studio della materia condensata.

Oggetto: Iniziativa Specifica LF-11

Partecipanti:

S. Bellucci, ricercatore INFN-LNF, 40% (anche su MI-12 al 60%)

M. Benfatto, ricercatore INFN-LNF, 100%

A. Di Cicco, Professore Associato (Incarico di Associazione LNF), 100%

R. Gunnella, Ricercatore Universitario (Incarico di Associazione LNF), 100%

C. Natoli, dirigente ricerca INFN-LNF, 100%, responsabile

A. Tenore, primo ricercatore INFN-LNF, 100%

Wu Z.Y., studioso straniero, Professore Ordinario (Incarico di Associazione LNF), 100%

Richieste per l'anno 2001 (cifre in ML): 10 (Inviti) 12 (Estero)

PROPOSAL

This research program aims at the theoretical analysis of strongly correlated electron systems. These include the layered cuprates and high T_c superconductors, the heavy fermion systems, the quasi one dimensional materials, the transition metal oxides and the nanostructures and mesoscopic structures, the fullerene clusters and lattices.

The enormous recent progress both in the art of sample preparation and in the measurement techniques has produced a wealth of high quality data on thermodynamic, transport and spectroscopic properties which often challenge the simple textbook interpretation. This is particularly true for materials showing evidence for strong electronic and magnetic correlation such as the materials mentioned above.

At the same time new non perturbative methods have been developed for dealing with strongly correlated systems, such as the Density Matrix Renormalization Group [1], the dynamical mean field theory [2] or the extension of the Lanczos technique to finite frequencies and temperatures [3].

The main goal is to apply these advanced theoretical methods to the field of strongly correlated electronic and magnetic systems and to confront the results with experimental data. Besides this, it is worth exploring older theoretical methods, like the equation of motion method for advanced/retarded Green Functions, to see whether all the potentialities of this technique have been exploited for the description of strongly correlated systems. At the same time methods borrowed from field theory and statistical mechanics will be used to bear on the description of the essential physics in such systems.

Possible areas of application

1. Doped Mott-Hubbard insulators

The main topics are still charge and spin fluctuations and their relation to superconductivity. Several studies have been concerned with the motion of a hole in an antiferromagnetic background, based on the t-J model or the spin-fermion model. This latter has been mapped onto a non linear sigma model in order to identify the low-lying degrees of freedom. We would like to investigate this aspect. Another very interesting field is the interpretation of the Fermi surface mapping by Aebi et al [4] of $\text{Bi}_2 \text{Sr}_2 \text{CaCu}_2 \text{O}_{8+x}$, who have confirmed the existence of flat bands near the Fermi surface and shown evidence of bands which have been interpreted as sign of short range antiferromagnetic spin fluctuations.

In this context and for the interpretation of these data, we would like to try a method for introducing charge and spin correlations based on an equation of motion method proposed by Natoli many years ago [5] followed by a decoupling procedure at the relevant order of the Coulomb interaction. This method would allow the realistic description of both aspects of the physics of correlated systems, namely correlation and itinerancy. A preliminary application of this method to introduce correlations in an Hubbard model has been given by Castellani, Natoli and Ranninger et al [6] to describe the antiferromagnetic insulating phase of V_2O_3 and has been shown substantially equivalent to the more modern LSDA + U method [7]. The idea is to go to next order of the equations of motion to introduce interparticle interaction in a mean field description. If successful, this approach would allow to bypass the t-J model and would lend itself to a description of the superconducting state by simply taking into account the non conservation of the number of particles in the decoupling procedure (breaking of global gauge invariance).

2. Itinerant ferromagnetism
It is still not clear how the ferromagnetism of the ion group elements can be described within a simple model of correlated electrons, especially after it has been recognized that a simple one-band Hubbard model, originally introduced to describe band ferromagnetism, has a non-ferromagnetic ground state in nearly the entire parameter space [8]. Clearly the existence of degenerate bands is necessary. We propose to apply the method described above for a realistic description of these materials.

3. Heavy Fermions

Two issues are currently debated, the breakdown of the Fermi liquid theory in some of these fully three-dimensional compounds and the sometimes puzzling magnetic behaviour at low temperatures, often connected with an unusual superconducting state. No particular effort will be made to contribute in this field, but we shall keep an eye open for cross-field fertilization.

4. Manganites

These materials have stimulated a great activity after the discovery of the colossal magnetoresistance at the ferromagnetic transition. Theoretically an important challenge is the coupling of spin and charge to lattice and orbital degrees of freedom [9]. The standard model (Kondo lattice model) is still believed to capture the essential physics, but recent experiments indicate that both the Jahn-Teller effect and the orbital degeneracy may have to be explicitly taken into account. An important discussion will thus be concerned with the modeling of these substances and the interpretation of various types of experiments. Recently we have clarified the origin of the anomalous X-ray diffraction signal at the K edge of Mn [10] in the parent compound $LaMnO_3$. We would like to pursue this line of interpretation of spectroscopies using synchrotron radiation utilizing our expertise in the field and the new method proposed above.

5. One-dimensional conductors and quantum wires

The concept of a Luttinger liquid is now well established for one-dimensional interacting electron systems, but it is much less clear to what extent it is applicable to experiments on quasi-one-dimensional materials. Thus the problem of coupled chains has been intensively studied recently. A similar problem arises in quantum wires where one has to deal with different transverse channels. Here a particularly striking phenomenon is the conductance quantization [11].

On the theoretical side we would like to tackle the problem of the renormalization of the Coulomb interaction in such systems, using the renormalization group approach, with a particular attention to the low-energy behaviour of the long-range interactions and the transition from a Fermi liquid to a Luttinger liquid phenomenology in going from a two-dimensional to an one-dimensional behaviour. The predicted effects can be quite interesting, depending on the filling level of the system [12,13]. The phenomenological implications of this study are relevant in the fullerene nanostructures (metallic carbon nanotubes with big transverse section). Preliminary results have been presented at the VI International Conference on path Integral from peV to TeV, Firenze, 25-29 Agosto 1998 [14].

6. Fullerene clusters and lattices

The fullerene clusters and lattices are the ground of interesting physical phenomena, which have mainly to do with their electronic properties. Some of them already stem from the particular features of the interaction in the graphite sheet. It has been shown that the electronic spectrum of the C_{60} and giant fullerenes can be understood from the frustration introduced by the pentagon rings in the honeycomb lattice [15]. The unconventional screening properties of the interaction inside the clusters [16] (which quite probably play an important role in the high- T_c superconductivity of the compounds)

have their origin in the renormalization of the Coulomb interaction in the graphite sheet [17]. Recent photoemission experiments have shown that the quasiparticle decay rate in graphite has a linear dependence on the frequency close to the Fermi energy [18]. These measurements are consistent with the marginal Fermi liquid behavior of the interaction, as explained in [19].

The purpose of the future research is to apply these developments to the study of the electronic properties of the tubular fullerenes. The introduction of gauge fields, as it has been done in [15],[20], may be very useful to explain the effect of dislocations in the lattice.

...of dislocations in the lattice.

In certain cases, these are known to produce metal/semiconductor junctions in a single nanotube [21]. It would be interesting to have a field theoretical model for the combined effect of several such dislocations. On the other hand, the marginal behavior of the interaction may leave also imprints at the lower dimension of the nanotubes. These may inherit some of the electronic properties of graphite, specially for large radius of the tubule. This makes the study of the crossover from the marginal Fermi liquid behavior to the regime of strong correlations in one dimension a very interesting matter of research.

- [1] S.R. White, Density matrix formulation for quantum renormalization groups, Phys. Rev. Lett. 69, 2863 (1992)
- [2] For a review, see A. Georges, G. Kotliar, W. Krauth and M. Rozenberg, Dynamical mean-field theory of strongly correlated fermion systems and the limit of infinite dimensions}, Rev. Mod. Phys. 68, 13 (1996)
- [3] J. Jaklic and P. Prelovsec, Lanczos method for the calculation of finite temperature quantities in correlated systems, Phys. Rev. B 49, 5065 (1994)
- [4] P. Aebi et al, Phys. Rev. Lett. 72, 2757 (1994)
- [5] F. Leoni and C.R. Natoli, Connection between the equation of motion and perturbation theory approach to the evaluation of double-time spin-Green Functions, J. Phys. C 3, 1462-1482 (1970)
- [6] C. Castellani, C.R. Natoli and J. Ranninger, Phys. Rev. B18, 4945-5013 (1978)
- [7] V. Asaninmov, J. Zaanen and O.K. Andersen, Phys. Rev. B 44, 943 (1991)
- [8] For a review see D. Vollhardt, Non perturbative approaches to magnetism in strongly correlated electron systems, Z. Phys. B (June 1997)
- [9] A.J. Millis, P.B. Littlewood and B.I. Shraiman, Double exchange alone does not explain the resistivity of $\text{La}_{1-x}\text{Sr}_x\text{MnO}_3$, Phys. Rev. Lett. 74, 5144 (1995)
- [10] M. Benfatto, Y. Joly and C.R. Natoli, Critical reexamination of the experimental evidence of orbital ordering in LaMnO_3 and $\text{La}_{0.5}\text{Sr}_{1.5}\text{MnO}_4$. Phys. Rev. Lett., in press.
- [11] For a recent review see N. Garcia and J.L. Costa-Kromer, Quantum-level phenomena in nanowires, Europhys. News 27, 89 (1996)
- [12] 1999 "On the Coulomb interaction in chiral-invariant one-dimensional electron system", S. Bellucci and J. Gonzalez, cond-mat/9903022, European Physical Journal B, in press.
- [13] 1998 "Renormalization of the Coulomb interaction in one-dimensional electron systems", S. Bellucci and J. Gonzalez, cond-mat/9802011, Physical Review B (submitted), (3 citations).
- [14] 1999 "Long-range interactions in a one-dimensional electron system", S. Bellucci, Proceedings of the 6th Conference on Path Integrals, (Florence, 25-29 August 1998), edited by R. Casalbuoni, R. Giachetti, V. Tognetti, R. Vaia, P. Verrucchi, page 363, hep-th/9810181, (1 citation).
- [15] J. Gonzalez, F. Guinea and M. A. H. Vozmediano, Phys. Rev. Lett. 69, 172 (1992).
- [16] J. Gonzalez and J. V. Alvarez, Phys. Rev. B53 (1996) 11729.
- [17] J. Gonzalez, F. Guinea and M. A. H. Vozmediano, Nucl. Phys. B424 (1994) 595.
- [18] S. Xu et al., Phys. Rev. Lett. 76, 483 (1996).
- [19] J. Gonzalez, F. Guinea and M. A. H. Vozmediano, Phys. Rev. Lett. 77, 3589 (1996); *ibid.* Phys. Rev. B59, 2474 (1999).
- [20] J. Gonzalez, F. Guinea and M. A. H. Vozmediano, Nucl. Phys. B406 (1993) 771.
- [21] L. Chico et al., Phys. Rev. Lett. 76, 971 (1996).

Esperimento

gruppo

Rappresentante nazionale

Struttura res. naz

nuovo continua

LF-11

4

C. NATOLI

L.N.F.

continua

STR.	ESPERIM.	Missioni interno	Inviti ospiti stran.	Missioni estero	Mater. di Cons.	Spes Sem	Tras. e Fac.	Pub. Scien.	Spese Calc	Aff. e Manut. App.	Mater. invent.	Costruz. apparati	TOTALE
L.N.F.	Personale												
	Ricercatori	7,0	Tecnologi			Tecnici			Servizi mesi uomo				
	FTE	5,9	FTE			FTE							
	Rapporti (FTE/numero) Ricercatori				0,84 Ricercatori+Tecnologi				0,84				
	LF-11		10	12									22
	di cui sj												
	Totals		10	12									22
di cui sj													
Richieste/(FTE ricercatori+tecnologi)				3,73									
TOTALI													
Totals		10	12										22
di cui sj													
Confronto con il modello EC4													
Mod. EC4 dati		10	12										22
Totals-Dati EC4													
Personale													
Ricercatori	7,0	Tecnologi			Tecnici			Servizi mesi uomo					
FTE	5,9	FTE			FTE								
Rapporti (FTE/numero) Ricercatori				0,84 Ricercatori+Tecnologi				0,84					
Richieste/(FTE ricercatori+tecnologi)				3,73									