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SUBJECT: Report of Foreign Assignment of Mark Rasolt, Senior Research Staff Member, Solid State Theory Section, Solid State Division, ORNL

TO: Alvin W. Trivelpiece

FROM: Mark Rasolt

PURPOSE: To continue collaboration with F. Perrot at the Centre Européen de Calcul Atomique et Moléculaire (CECAM), University of Paris, Orsay, France, and to organize an International Meeting on High- T_c Superconductivity.

SITES VISITED: 4/12-8/28/90 Centre Européen de Calcul Atomique F. Perrot
et Moléculaire (CECAM), University
of Paris, Orsay, France

6/7-8/90 Service de Physique Theoretique J. Zinn-Justin
Saclay, Gif-sur-Yvette, France

ABSTRACT: A detailed description of the research conducted at the University of Paris at Orsay and the International Meeting on High- T_c Superconductivity, organized by the traveler, H. Schultz from Orsay, and D. M. Newns from IBM, is presented. Particular emphasis is placed on the collaboration with F. Perrot of the Centre Européen de Calcul Atomique et Moléculaire. In addition, descriptions of the different scientific interactions and information obtained and implications of this scientific exchange on the research conducted in the Solid State Division of ORNL are made.

I. INTRODUCTION

The traveler was invited to spend three months at the Centre Européen de Calcul Atomique et Moléculaire (CECAM), University of Paris, Orsay, France, and to help organize an international meeting on high- T_c superconductivity entitled "Analytical Versus Numerical Treatments of Models for High- T_c Superconductivity." The trip had dual objectives: (1) to continue collaboration with F. Perrot on various projects of interest to ORNL and to the traveler and to open new areas of collaboration, primarily in high- T_c superconductivity, and (2) to cochair an international meeting on the theory of high- T_c superconductivity whose purpose was to help develop stronger links between analytic and numerical techniques for solving some of the existing models, which are candidates for explaining the microscopic mechanism of high- T_c superconductivity.

These two objectives were very successful. The collaboration with F. Perrot has produced new and important research directions in high- T_c superconductivity. The international meeting led to some very important exchange of ideas in high- T_c superconductivity, has brought some new insight to the traveler, and enhanced the reputation of ORNL in this exciting field.

The following sections detail the collaboration with F. Perrot and Z. Tesanovic and the interaction at the international workshop.

II. SCIENTIFIC COLLABORATION WITH F. PERROT AT ORSAY

The main collaboration at Orsay is a continuation of my work with F. Perrot. Perrot has developed numerical expertise which is of central importance to the traveler's research. Perrot's fields of expertise include the development of numerical codes for calculating charge densities of complicated defect geometries and the corresponding total energy calculations of such configurations, charge densities at metal surfaces and the corresponding screening and pair interactions, pair correlation functions and the corresponding thermodynamic properties of a two-component plasma of electrons and ions, and self-consistent band-structure calculations. It is his expertise in band-structure calculations which was primarily exploited during

this collaboration, in application to high- T_c superconductivity. We have also continued our research on highly excited classical plasmas and free electron-like density in complicated band structures.

A. Chiral Spin Liquid State and the Corresponding Anyons, as a Mechanism for High- T_c Superconductivity

One of the exciting proposals for the mechanism of high T_c is the creation of "particles" with fractional statistics called anyons. The existence of these anyons depends crucially on the two dimensionality of the Cu-O planes and the existence of a particular gauge field whose origin is the spontaneously broken symmetry of the ground state; so-called chiral spin liquid. It has been assumed that such a chiral ground state can exist in the high- T_c materials; three available experiments give conflicting results. Following such an assumption, the scenario of anyon superconductivity is very plausible. The fractional statistics places the carriers between fermions and bosons leading to a real space-like condensation (not unlike the Bose condensation of He^4), which could require no pairing mechanism. More precisely, the fractional statistics can be mapped to another gauge field (called the Chern Simon field) which shares similarities with a spontaneously created uniform magnetic field leading to many of the properties shared by the quantum Hall effect.

In a recent issue of *Physical Review Letters* [65, 1498 (1990)], the traveler presented a rigorous formulation of this self-induced gauge field which gives an exact form for its spatial structure and shows that it cannot support an anyon gas in the Cu-O plane. Therefore, it is unlikely that anyons are responsible for high- T_c superconductivity. There remains, nevertheless, some important issues. For example, can the strong correlations within the copper-oxygen (Cu-O) planes of high- T_c perovskites produce spontaneously induced persistent currents, not unlike those observed in He^3 ? The formulation described above is ideal for tackling this important problem.

The difficulty of the numerical aspect of the calculation is that it requires a self-consistent band-structure code, which includes not only the self-consistent density but self-consistent currents as well. F. Perrot and the traveler have developed (to our knowledge) the first such band-structure code. Even though the code is simplified by the two dimensionality of the Cu-O planes, its development turned out to be a very nontrivial numerical task. We

are now beginning to search for the possibility of a self-induced current-carrying ground state in the Cu-O plane. In future collaborations we intend to extend this code to three dimensions. It will then be possible to look at, for example, quantum wells in very strong magnetic fields and other interesting phenomena in the new frontiers of semiconductor technology.

B. Highly Excited Classical Plasma

We have continued calculations in highly excited plasmas. The traveler and F. Perrot have published in *Physical Review Letters* [62, 2273 (1989)] showing that classical plasmas far away from equilibrium, with densities an order of magnitude higher than the corresponding solid density, can have a new rapid recombination channel. This happens when the excited plasma density and the corresponding plasma frequency can match the transition energy to the core levels. Such highly excited densities exist commonly in attempts at fusion of the plasma. In our previous calculations, we ignored the width of the core levels and applied our theory to light metals such as aluminum. We now have codes which include the core level's lifetime, and we are extending our applications to the heavy element classical plasmas.

C. Free Electron-Like Density in Complicated Band Structure

A complicated metal (e.g., palladium) has a mixture of s,p-like bands and the more localized d bands. The free electron-like s,p bands are highly extended, and it is very useful to identify a procedure for extracting them. We have found such a numerical procedure and have now completed a continuation of our calculation by extracting this s,p contribution in both the 3d and 4d transition series. A paper is in preparation.

III. SCIENTIFIC COLLABORATION WITH Z. TESANOVIC AT ORSAY

Z. Tesanovic, from Johns Hopkins University, came to spend a couple of weeks at Orsay to continue collaboration with the traveler. Tesanovic and the traveler started collaborating when the traveler was visiting B. I. Halperin (1987) at Harvard University; Tesanovic was Halperin's postdoctorate student.

At Orsay we collaborated in two areas: (1) superconductivity enhanced by strong magnetic fields and (2) a charge redistribution approach to superconductivity in YBCO/PBCO superlattices.

A. Superconductivity Enhanced by Strong Magnetic Fields

In *Physical Review Letters* [58, 1482 (1987)], the traveler showed that for multivalley doped semiconductors the electron spin can be replaced by the valley components. The traveler proposed a novel superconducting state which suffers no Pauli (spin) breaking and can be enhanced in the presence of a strong magnetic field. Following this suggestion, the traveler and Tesanovic in *Physical Review Letters* [63, 2428 (1989)] showed how this state can exist in low carrier density semimetals and semiconductors even for real spins. Our collaboration at Orsay continued to develop further the application of this new state to systems with various Zeeman splittings and to the study of the effect of impurities. We showed, without any doubt, that the effect of Zeeman pair breaking and a reasonable density of impurities do not seriously affect the stability of this state in the high magnetic limit where both spins are occupied and reside in the lowest Landau level.

B. A Charge Redistribution Approach to Superconductivity in YBCO/PBCO Superlattices

In two recent *Physical Review Letters* by A. Li et al. [64, 3086 (1990)] and D. H. Lowndes et al. [65, 1160 (1990)], alternating layers of $\text{YBa}_2\text{Cu}_3\text{O}_{7-x}/\text{PrBa}_2\text{Cu}_3\text{O}_{7-x}$ have been studied. The critical temperature was determined as a function of YBCO layer separation and thickness. We propose using such experiments to understand some fundamental issues in critical fluctuations in two dimensions (Kosterlitz-Thouless) and the crossover to three dimension. In order to identify the features of these experiments which reflect the Kosterlitz-Thouless phase transition and the crossover to three dimensions, the effect of charge redistribution must be removed. A simple model for the superlattice has been constructed, and the functional density theory has been applied to calculate this charge redistribution. The trend of the experiments is reproduced, but much more important, we are convinced that once this charge redistribution is removed, there still remains a strong

signature of the critical fluctuations. The electronic calculation is being refined as a next step. We then hope to recommend further experiments in the direction of Kosterlitz-Thouless and crossover behavior.

IV. INTERNATIONAL MEETING ON HIGH- T_c SUPERCONDUCTIVITY

The traveler invited 20 of the leading theorists in high- T_c superconductivity for a two-week meeting at Orsay. The theorists represented just about all the facets of recently proposed models, which could potentially explain the microscopic mechanism of high- T_c superconductivity. Furthermore, the organizers tried to achieve a balance between theorists who use numerical simulations and analytical techniques. The purpose was to merge the two approaches, which have unfortunately largely been evolving separately.

I next list the talks presented and a brief summary.

- (1) C. M. Varma, AT&T Bell Laboratories, spoke on "Marginal Fermi Liquids." Varma's primary point is that the linear dependence of the resistivity on temperature above the superconducting transition reflects deviation from a true Fermi liquid.
- (2) D. M. Newns, IBM Yorktown Heights, spoke on "High- T_c Superconductors Light Mass Heavy Fermion Systems." Newns (and the traveler) feel that the system above the superconducting transition is a highly correlated but standard Fermi liquid.
- (3) M. Imada, University of Tokyo, spoke on "Numerical Simulations of the Hubbard Model." Imada from his numerical simulations finds that away from a half-filled Hubbard band (i.e., a half-filled Cu-O plane), the insulating antiferromagnetic Neél state is unstable.
- (4) G. Kotliar, Rutgers University, spoke on "Field Theoretical Treatment of the t-J Model." Kotliar considered new states within the t-J model in which charge and spin degrees of freedom separate (i.e., holons and spinons in RVB language), which account for much of the optical properties of the perovskites above the superconducting transition.

- (5) M. Rasolt, Oak Ridge National Laboratory, Oak Ridge, Tennessee, spoke on "Self-Induced Gauge Fields in the Cu-O Planes of High- T_c Perovskites." The traveler showed that the self-induced gauge field cannot support an anyon gas (see Section II.A).

V. SERVICE DE PHYSIQUE THEORETIQUE SACLAY, GIF-SUR-YVETTE, FRANCE

The traveler was invited to the Service de Physique Theoretique Saclay, Gif-Sur-Yvette, France, to speak on "Self-Induced Gauge Fields in the Cu-O Planes of High- T_c Perovskites: A Lattice and a Continuum Formulation" and to discuss some aspects of critical phenomena with one of the leading field theorists, J. Zinn-Justin. The lecture was well-received, and the discussion with Zinn-Justin brought some new ideas in the field of helium in Vycor, an area of long-standing interest to the traveler.

VI. CONCLUDING REMARKS

The traveler views this assignment as very important to his research and to the interest of ORNL. The collaboration with F. Perrot has been continued and extended to high- T_c superconductivity. F. Perrot's expertise in various areas of condensed matter physics has been crucial to the traveler and could become useful to ORNL in more general problems of solid state physics. This collaboration and its continuation are very important to me and to ORNL.

Finally, the exchange of information with a wide range of scientists and the lectures presented brought new ideas and contacts important both to me and to other colleagues at ORNL.

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APPENDIX A

ITINERARY

DATES	LOCATION	INDIVIDUALS CONTACTED	SUBJECT OF DISCUSSION
4/12/90	Travel en route from Oak Ridge, TN, to Paris, France, via plane		
4/16-6/6/90 6/9-7/9/90 8/8-27/90	Centre Européen de Calcul Atomique et Moléculaire, University of Paris, Orsay, France	F. Guinea D. Hewson M. Imada G. Kotliar H. R. Krishnamurthy M. Lavagna I. Morgenstern C. Moser D. M. Newns P. C. Pattnaik F. Perrot G. Sawatzky H. Schulz S. Sorella Z. Tesanovic C. M. Varma W. Von der Linden J. Zaanen	To collaborate with F. Perrot and Z. Tesanovic on superconductivity, stability of highly excited plasmas, and charge densities in complex band structures; to organize an International Meeting on High-Temperature Superconductors, and to present a lecture.
6/7-8/90	Service de Physique Théoretique Saclay, Gif-sur-Yvette, France	J. Zinn-Justin	Present seminar

APPENDIX A (Cont'd)

ITINERARY

DATES	LOCATION	INDIVIDUALS CONTACTED	SUBJECT OF DISCUSSION
7/10-8/7/90	Vacation		
8/28/90	Travel en route from Paris, France, to Sacramento, CA, via plane		

END

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10 / 31 / 90