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Final Report
Superconducting Materials

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Papers Published During Grant Period

1. " Hall Effect and Electronic Structure of $La_{2-x}Sr_xCuO_4$ ", J.Ruvalds and A. Virosztek, Phys . Rev. B42, 399(1990)

2. " Infrared Reflectivity of High T_c Superconductors ", J. Ruvalds and A. Virosztek, Physica B165, 1267 (1990)

3. " Nested Fermi Liquid Theory ", A. Virosztek and J. Ruvalds, Phys. Rev. B42, 4064 (1990)

4. " Optical Properties and Fermi Surface Nesting in Superconducting Oxides "' J. Ruvalds and A. Virosztek, Phys. Rev. B43, 5498 (1991)

5. " Superconductivity in $Ba_4BiPb_2TlO_{12}$ ", T.E.Sutto, B.A.Averill and J. Ruvalds, Chemistry of Materials 3, 209 (1991)

6. " Raman Scattering by a Nested Fermi Surface ", A. Virosztek and J. Ruvalds, Phys. Rev. B. 67, 1657 (1991)

7 " Raman Spectrum of Superconducting Oxides ", A. Virosztek and J. Ruvalds, Phys. Rev.B45, 347 (1992)

8. " Fermi Surface Nesting in High Temperature Superconductors ", J. Ruvalds, J. Zhang, and A. Virosztek, J. Phys. Chem. Solids 52, 1371 (1991)

9. " Spin Susceptibility Scaling in High-Temperature Superconductors ", J. Ruvalds, J.Zhang, and A. Virosztek, Science 256, 1664 (1992)

10. " Acoustic Plasmons and Cuprate Superconductivity ",Y.Ishii and J. Ruvalds, Phys. RevB48,3455(1993)

11."Conductivity below T_c in High Temperature Superconductors",C.T.Rieck, W.A.Little, J.Ruvalds, and A.Virosztek,PhysicaB194,1465 (1993)

12."Energy Gap, Susceptibility, and Damping in High Temperature Superconductors" C.T.Rieck, W.A.Little, J.Ruvalds, and A.Virosztek, Sol.St.Comm.88,395(1993)

13. "Conductivity Below T_c in High Temperature Superconductors", C.T.Rieck, W.A.Little and A.Virosztek, Physica B194,1465(1994)

14. " Nesting Mechanism for d-symmetry Superconductors ", J.Ruvalds, C.T. Rieck, S. Tewari, J.Thoma, and A. Virosztek , Physical Review B 51,3797(1995).

15. " Infrared and Microwave Spectra of an Energy Gap in High Temperature Superconductors " C.T.Rieck, W.A. Little, J.Ruvalds and A. Virosztek , Physical Review B51, 3772(1995).

16." Susceptibility and Knight Shift Anomalies in Cuprate Superconductors ", J. Thoma, S. Tewari, J.Ruvalds, and C.T.Rieck, Physical Review B51,15,393(1995)

17. "Fermi Liquid Damping and NMR Relaxation in Superconductors", S.Tewari and J.Ruvalds, Phys.Rev.B53,5695(1996)

18. "Optical Spectra of High Temperature Superconductors", J.Ruvalds, in Spectroscopic Studies of Superconductors (SPIE Volume 2696),108(1996)

19. "Theory prospects for High Temperature Superconductors", J.Ruvalds, Superconductor Science and Technology **9**,905(1996)

20. "NMR Spectra in High Temperature Superconductors", D.Djajaputra and J.Ruvalds, Phys. Rev. B**55**, 14,148(1997)

21."Susceptibility and vertex corrections for a square Fermi surface", D.Djajaputra and J. Ruvalds, Int. J. Mod. Phys. **B13**,25(1999)

22. "On the Hubbard Model at Half Filling", D.Djajaputra and J. Ruvalds, Solid State Communications **108**, 899(1999)

23 ."Susceptibility scaling and vertex corrections for a nested Fermi liquid", A.Virosztek and J.Ruvalds, Phys. Rev. B**59**,1324(1999)

24. "Spin susceptibility divergence in high-temperature superconductors", D.Djajaputra and J .Ruvalds, Sol. State. Comm.**111**,199(1999)

25. "Microwave spectra of d-wave superconductors", C.T Rieck and J.Ruvalds, Phys. Rev **60**, ... (October, 1999)

Invited Talks

1990

IBM Thomas J. Watson Research Center
Gordon Conference on Correlated Systems, Brewster, MA
Universite Pierre et Marie Curie, Paris. Institut Laue-Langevin, Grenoble, France
Kernforschungszentrum, Karlsruhe, Germany.Walther-Meissner Institut, Garching, Germany.University of California, Irvine. University of California, Los Angeles

1991

Fermiology Workshop on Superconductors, Argonne; University of Toronto, Los Alamos National Lab, Stanford University, Southeastern Meeting of the A P S, Durham, NC

1992

U. of Illinois Spin Workshop, Urbana, IL, Los Alamos National Lab

1993

Gordon Conference on Superconductivity, Oxnard, CA (Jan., 1993)
University of California, Davis,CA

1994

Chalmers Institute of Technology, Goteborg, Sweden
Daugavpils Pedagogical University, Latvia; Institute of Solid State Physics, Riga, Latvia
Niels Bohr Institute, Copenhagen, Denmark

1995

University of Maryland. Technical University of Budapest, Hungary
UCLA Workshop on non-Fermi Liquids. AtomInstitut Vienna, Austria
Charles University,Prague,Czechoslovakia. Institute for Solid State Physics, Riga, Latvia
NORDITA Conference on 2D Electron Gas, Copenhagen, Denmark

1996

SPIE Conference on Spectroscopic Studies of Superconductors, San Jose, CA

1997

University of Missouri, University of Hamburg, Wurzburg University, Walther Meissner Institut (Garching, Germany), Max Planck Institut fur Komplexer Systeme (Dresden), Institute for Solid State Physics (Riga, Latvia); Freie Universitat Berlin (Germany)

1998

Louisiana State University, New 3SC Conference on High Temperature Superconductors, Baton Rouge, LA

1999

Los Alamos National Lab; University of California (UCSD) La Jolla,CA

Graduate Students and Personnel

Graduate student David Djajaputra won the **Gwathmey** prize for the best thesis research at the University of Virginia. His 1999 PhD thesis on superconductors was also honored by the **Z society** award for outstanding contributions to academic vigor at the University. He is the best graduate student that I have encountered in our department in the last twenty years. His motivation, dedication to science, and mathematical skills are on par with the top 1% of postdoctoral candidates that I have interviewed from the best Universities in the USA. His discovery of an important theorem for a Hubbard model at half-filling received many congratulations from experts in the scientific community this year. His discovery of a new many body effect – in the form of a divergent spin susceptibility – for interacting electrons on a nested Fermi surface has attracted favorable comments, especially since the effect has been observed by neutron scattering from high temperature superconductors and a metallic vanadium oxide.

David received several job offers and chose to join the theory group of Prof. B. Cooper at the University of West Virginia as a research associate.

Dr. A. Virosztek completed his postdoctoral appointment in our group in the summer of 1990 and now interacts with our group from Budapest. He won two prizes from the Hungarian Academy of Sciences in recognition of his work at Virginia. His recent research on vertex corrections justifies key features of our nesting theory, and reveals significant corrections to the standard random phase approximation (RPA).

Dr. Shubha Tewari joined our group as a research associate after completing her PhD thesis at UCLA. Her research at Virginia began in 1993, and led to the development of a new theoretical explanation for high superconducting transition temperatures. She completed her term at Virginia in 1996 and is now teaching in Massachusetts.

Dr. Carsten Rieck was a Research associate in our group until 1993. He recently completed a study at the University of Hamburg of infrared and microwave properties of superconductors, which has been accepted for publication in Physical Review B.

Time Devoted to Project by Principal Investigator

1. 50% of time during academic year period April 1, 1999 to May 31, 1999

2. 100% of time June 1 , 1999 - August 31, 1999

3. 50 % of time during academic year period September 1, 1998 to March 31, 1999

Synopsis of Research

Our group discovered an electronic mechanism for creating superconductivity at high temperatures in metals that have "nested" Fermi surfaces in the form of nearly parallel orbit segments. We also found that nested electron collisions explain the unconventional optical properties which distinguish cuprate superconductors from ordinary metals.

Fundamental progress on higher order corrections to the susceptibility of a nested surface was achieved by our group. We proved that self energy and vertex corrections preserve the surprising scaling of the spin susceptibility, which is the key nesting feature that explains various properties of high temperature superconductors. We also discovered significant corrections to the standard random phase approximation (RPA).

We proved a theorem for a half-filled Hubbard model which substantially reduces the task of computing higher order corrections to the susceptibility. By virtue of particle-hole symmetry, this theorem shows that diagrams with loops containing an odd number of particle lines cancel the corresponding processes with hole lines. Thus a large number of graphs can be neglected when energy bands are nearly half-filled, a scenario that is realized in high temperature superconductors.

A breakthrough in the above analysis led our group to discover a new many body effect, which yields a power law divergence of the static spin susceptibility – at a nesting vector – as a function of temperature. Using a Parquet method, we proved the effect for a Hubbard model to all orders in the Coulomb repulsion U. The effect has been observed in a high temperature superconductor and also in metallic vanadium oxide.

Our computations of the microwave spectra in cuprate superconductors improve the fundamental understanding of the dramatic drop of the damping in the superconducting state. This reduced collision rate enhances quality factors in superconducting devices and benefits communications technology in the microwave range.

I. Nesting Mechanism for High Temperature Superconductors

We discovered that Fermi surface nesting significantly strengthens the d-wave pairing of electrons. In contrast to the conventional BCS theory that relies on phonon exchange to pair electrons in a s-state, the d-symmetry pairing is caused by a Coulomb repulsion.

The concept of superconducting electrons that are paired via the exchange of charge or spin fluctuations was explored more than thirty years ago, but estimates for a standard spherical Fermi surface gave discouraging low values of the transition temperature.[1]

Stimulated by the unconventional nature of the energy gap symmetry in heavy Fermion metals and cuprates, many groups have investigated the spin fluctuation pairing in tight-binding models.[2] Generally such calculations yield a very weak pairing in leading order, so some theorists use the random phase approximation (RPA) series to raise the transition temperature. However, Schrieffer[3] has argued that vertex corrections may offset the RPA enhancement. We found that vertex terms are indeed an essential element in our nesting theory, and we are pleased to report our recent analysis of a general theorem in section II and a study of logarithmic divergences in section III.

We found[4] that superconducting transition temperatures of 100 K can be achieved for a nested surface in leading order, when the nesting vector is within a narrow range. Our Fermi surface modeled the nesting features of Bi2212 that were measured by the Stanford photemission experiments.[5,6]

Our recent results for the superconducting transition temperature link the high T_c values to the unconventional optical properties of cuprates, which we explained in terms of electron collisions on a nested surface[7,8]. Small changes in oxygen content typically depress T_c and simultaneously eliminate the anomalous damping features in cuprates - in accord with the expectation of nesting changes caused by chemical composition.

An invited review article on superconductors for non-specialists was completed and appeared in print recently.[9]

Using a Hubbard on-site Coulomb repulsion U and a tight binding energy band model with nesting features that are similar to the photoemission data for Bi2212, we discovered that the calculated superconducting transition temperature T_C varies with the nesting vector **Q***, as shown in Figure 1. The solid calculated curve intersects the known value of T_C = 85K for Bi2212 for a value of U that is comparable to the bandwidth. A smaller nesting vector - like the value for Bi2201 seen by photo-emission spectra [6] - reduces T_C dramatically, in accord with experiment. The Fermi liquid case (a rounded orbit without nesting) gives T_C=0 within this leading order calculation. If the nesting vector enters the shaded region close to the half-filled band case, a SDW regime [10] dominates.

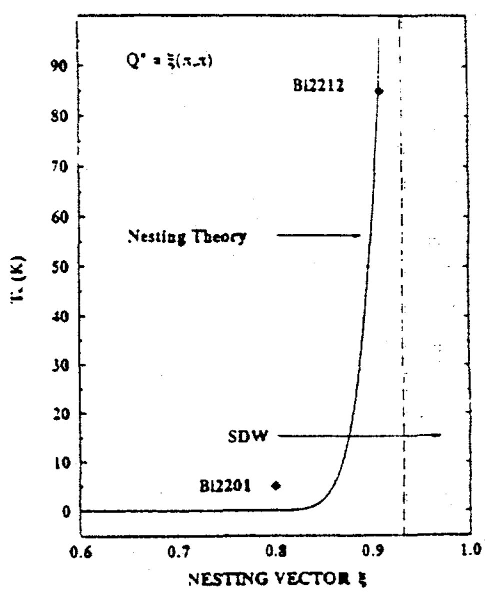

Figure 1. Calculated superconducting transition temperature for a d-wave state reveals a strong variation with the nesting vector **Q*** as seen for the solid curve. A match to the experimental T_C for Bi2212 is achieved in leading order for a value of the Coulomb repulsion U that avoids the SDW instability. Decreasing the nesting vector reduces T_C and thus explains the low value for Bi2201, while larger values of **Q*** trigger a spin density wave within the shaded region.

Encouraged by these results, we examined higher order self energy and vertex corrections to the susceptibility. This path led to the proof of a novel theorem and the discovery of a new many body effect.

II. Theorem for a Hubbard model

The Hubbard Hamiltonian is defined by

$$H = \sum_{k,\sigma} \varepsilon(k) c_{k,\sigma}^{+} c_{k,\sigma} + U \sum_{r} (n_{r\uparrow} - 1/2)(n_{r\downarrow} - 1/2)\,, \qquad (1)$$

where $\varepsilon(k)$ is the electron energy, U is the on-site Coulomb repulsion, $c_{k,\sigma}$ is the destruction operator for a quasi-particle with momentum k and spin σ, and $n_{r\sigma}$ is the occupation operator at site r. This has become a standard model for high temperature superconductors. Many theoretical approaches have examined various types of energy band dispersion models. For highly correlated electrons, the basic many body problem is complicated by the large number of diagrams that are generated in all orders of U.

Our research has emphasized new features emanating from the nesting condition

$$\varepsilon(k+Q) + \varepsilon(k) = 2\mu \qquad (2)$$

where Q defines the nesting vector and μ is the Fermi energy. Given this condition, the lowest order non-interacting susceptibility χ , i.e. a particle-hole "bubble" , exhibits a logarithmic divergence at low temperature T and frequency ω. Hence higher order self energy and vertex corrections will diverge with progressively higher powers of functions containing terms like the log (max[T,ω]).

Nesting is traditionally associated with spin density waves, and the theoretical treatment of Chromium exhibits many remarkable features of the above divergences which invalidate traditional Hartree-Fock and random phase (RPA) approximations.[11]

Noting that the energy bands of high temperature superconductors are typically close to half-filling, we examined the case of perfect nesting with particle - hole symmetry and we proved[12] the following theorem: For a Hubbard model at half-filling, diagrams which have a loop consisting of an odd number of propagators are cancelled exactly by their partner diagrams which have the direction of all propagators in the loop reversed. These diagrams can therefore be omitted from the perturbation analysis of the model.

This theorem is relevant to high temperature superconductors where the Hubbard model is often used to study the competition between antiferromagnetic spin ordering and d-wave superconductivity that occurs close to half filling.

An example of diagrams that cancel each other is shown in Figure 2. Even these second order graphs are troublesome to evaluate otherwise, and the value of the theorem naturally becomes progressively more important in higher orders.

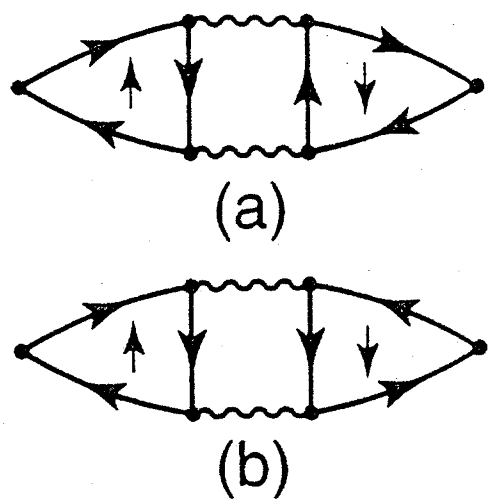

Figure 2. These two diagrams have loops consisting of odd number of propagators with lines running in opposite directions and wavy lines for the Coulomb repulsion U. At half filling these graphs exactly cancel each other.

Our proof of this theorem uses the well known Lieb-Mattis transformation and has been published[12]. Although our result is analogous to the Furry theorem in quantum electrodynamics, the nesting requirement has no analog in QED. In condensed matter physics, a theorem for the Anderson model derived by Iche and Zawadowski[13] involves similar symmetry transformations for the Green's functions and greatly simplifies the many body theory in that case.

The present result for the Hubbard model has already proven to be useful by eliminating the above diagrams from an analytic derivation of self energy and vertex corrections to the susceptibility which lead to a new many body effect.

III. New many body effect in superconductors and metallic oxides.

A surprising scaling of the spin susceptibility was discovered by our group for non-interacting electrons whose energy satisfies the nesting condition in Equation 2. This scaling as a function of frequency/ temperature (ω/T) is apparent in the "bare' nested Fermi liquid (NFL) susceptibility[9]

$$\Pi''_{NFL,0} = \frac{\pi N(0)}{2} \tanh[\omega / 4T] \qquad (3)$$

where N(0) is the density of electron states at the Fermi energy. The above basic scaling features have been verified[9] by neutron scattering experiments on large superconducting cuprate crystals at Grenoble, Brookhaven and Oak Ridge.

From the theoretical point of view, the above form of the scaling provides a physical explanation for the anomalous collision damping that distinguishes cuprates from ordinary metals (the latter have a Fermi liquid weak scattering). However difficulties arise because there is an associated logarithmic divergence in the real part of the nested susceptibility. Higher order corrections contain similar logarithmic divergences.

To resolve these issues we calculated analytically the self energy and vertex corrections to the susceptibility by including terms of second order in the Coulomb U. The main result of this theoretical advance is a proof that scaling of the susceptibility is preserved despite quantitative corrections to the form of the susceptibility.[14] Although this proof is quite general, the technical details are complex and available in a reprint.

Analytic derivations of the susceptibility in the static limit ω = 0 were achieved in logarithmic accuracy, and these results display crucial corrections to the standard random phase approximation (RPA) which is commonly applied in the field of superconductivity. The total spin susceptibility to second order in U then becomes

$$\chi'_{NFL}(Q, \omega = 0) = 2\chi_0[1 + U\chi_0 + \frac{2}{3}U^2\chi_0^2] \qquad (4)$$

where the bare susceptibility is

$$\chi_0 = N(0)\ln[D/T] \qquad (5)$$

and D is a cut-off energy of the order of the bandwidth. Clearly the vertex corrections invalidate the geometric RPA series already in second order in the Coulomb coupling.

Our independent calculations[15] for a square Fermi surface model verify the essential nature of the vertex corrections at the nesting vector , while providing a basis for future studies at arbitrary momenta.

Inspired by the above progress, we discovered a remarkable many body effect that appears as a power law divergence of the spin susceptibility as a function of temperature. Our theory yields the solid curve in Figure 3, which fits the neutron scattering data[17] on the LSCO superconductor quite well.

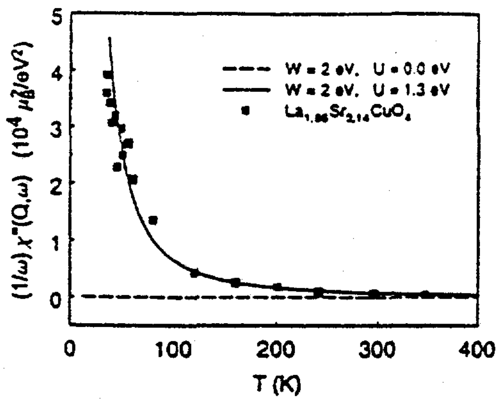

Figure 3. The imaginary part of the transverse spin susceptibility at a nesting vector Q displays a power law divergence as a function of temperature T. At low frequency the neutron data squares were measured on the LSCO cuprate, whereas the solid curve shows our calculated result for a value of the Coulomb U that is comparable to the bandwidth.

Our group solved the vertex correction problem to all orders in the Coulomb interaction by means of the Parquet method. The analysis predicts an asymptotic relation between non-universal exponents for the T and ω variation of the susceptibility, which should be observable in many metals with nesting. Thus we were glad to learn that neutron scattering experiments[18] on metallic V_2O_3 confirm the existence of a divergent susceptibility with exponents that conform to our prediction.

IV. Microwave Spectra of Superconductors

Communications and sensor technologies benefit from the optical response of copper oxide alloys in the superconducting state. The ultra-low surface resistance of these superconductors at liquid nitrogen temperature enables the design and fabrication of circuits and filters with high quality factors and negligible energy loss. Theoretical understanding of the damping processes that determine the resistance is useful for electronic design, and provides insight into the fundamental physics of the cuprates.

The cuprate infrared reflectivity deviates sharply from the conventional Drude behavior that characterizes conventional metals . Our nested Fermi liquid (NFL) calculations of the conductivity[8] describe the experiments above Tc very well, and now we have generalized the theory to describe a d-wave energy gap in the superconducting state.

An energy gap depletes the available scattering states for electron collisions and thus suppresses the damping in a distinct fashion that depends on the symmetry and magnitude of the gap. Our calculations[19] of the collision damping in the presence of an isotropic s-wave energy gap yield a very sharp decrease in the NFL damping and surface resistance below Tc, but the exponential drop at very low T falls below the microwave data on YBCO measured by Hardy's group[20].

Recently we extended our nesting formalism to incorporate an anisotropic d-wave gap, which is a natural choice for pairing via a Coulomb interaction. The d-wave gap symmetry is supported by elegant experiments on copper oxide superconductors.[9]

The theoretical analytic derivations and numerical integration which are available in a manuscript[21] that will be published in Physical Review B next month. Thus we report only the primary conclusions.

Our calculations[21] of the infrared conductivity as a function of frequency show that a d-wave gap is well suited to the experimental data of Basov et al[22]. The d-wave gap and collision damping on a nested surface produce strength at low frequencies that extends to the maximum value of the gap and then matches the normal state conductivity which falls off as ω^{-1}. Although other groups have computed the conductivity for tight-binding models with a similar d-wave gap, their choices of Fermi surface topology are appropriate to a Fermi liquid damping which gives quite a different behavior for the normal state.

Our results for the microwave surface resistance are shown in Figure 4 in comparison to the data[20] of Hardy's group. The remarkable drop in Rs just below Tc is a consequence of diminished damping and a strong coupling gap value. At intermediate temperatures the semilog scale of the drawing exagerates the discrepancy between theory and experiment, although it is reassuring that more recent microwave experiments by Hardy's group actually show the slight curvature in Rs displayed by the solid curve.

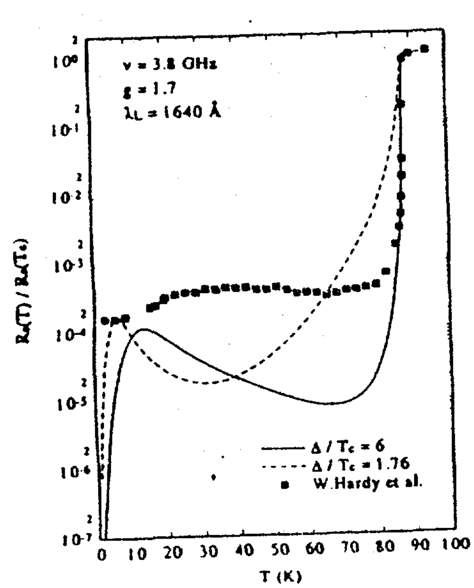

Figure 4. Microwave surface resistance data points from reference 20 show that R_s drops by four orders of magnitude when T is below the superconducting T_c=92K of YBCO. Our nesting calculations yield the curves for a d-wave energy gap, which give a better fit for a large gap value.

Thus we conclude our research with results for infrared and microwave spectra that are relevant to internet communications technology.

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5. 5. Z.X. Shen et al , Phys. Rev. Lett. **70**,1553(1993) and references cited therein.

6. D.M.King et al, Phys. Rev. Lett.**73**,3298(1994)

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16. D.Djajaputra and J.Ruvalds, Solid State Comm.**111**,199(1999)

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20. W.A.Bonn et al, Phys.Rev.**B47**,11,314(1993)

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22. D.N. Basov et al, Phys.Rev.Lett. **74**, 598(1995)