Computer Simulation Study of High T(c) Superconductor Structure

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I. A Major Success

The project funded by AFOSR under the grant 91-0337 for the past three and a half of years has reached a brilliant achievement in understanding the mechanism of high-temperature superconductivity (HTSC). A basic theory describing the mechanism and origin of HTSC has been established. It is not completely finished, but the outline and kernel of the theory have been done. This is a revolutionary breakthrough in seeking the mechanism of HTSC that is entirely different from the currently prevailing theories and models.

The main point of this theory lies in the mechanism of superconductivity in high-temperature superconductors (HTSC's) or the origin of the attractive interaction between two electrons in a Cooper pair. It is said in the theory developed in the present project that the origin of attraction between two electrons in HTSC's stems from the Coulomb-type interaction due to the electron correlation effects enhanced by the layered spatial structure. In other words, the superconductivity in HTSC's is induced by the electron-electron correlations. In contrast to the viewpoint of electron-phonon interaction mechanism of superconductivity, stemming from the BCS theory, the new viewpoint is that the electron-electron interaction mediated by electron-hole excitations governs behaviors of HTSC.
Of more importance is that this theory shows the possibility to unify the BCS theory, which is valid for the conventional superconductivity, and the theory of HTSC. Of course, more work is needed to make a conclusion.

Although the overall recognition has not been made yet, it will certainly be accepted and admitted one day by the community of superconductivity that the theory developed by the PI and his assistant in this project is only correct.

II. Technical Accomplishments

The accomplishments during the period of 3.5 years include the following;

A) Discovery of Microscopic Two-Body (Pair) Interaction Potential in a Layered Two-Dimensional (2D) System

As done by many other scientists in the molecular-dynamics (MD) simulation study, the phenomenological study was first tried in acquisition of interaction potential, but it was not successful. Therefore, the effort turned to the theoretical investigation to search for a formalism of the microscopic interaction. This is the most successful and fundamental work in the present project. Without this success there would be no further motivation to switch our efforts at once to acquiring the mechanism of HTSC.

The pair interaction potential between two electrons (holes), shown in Fig. 1, presents a negative part within a certain range of interparticle distances which implies that two electrons could attract each other to form a stable bond state. In contrast to the mechanism of a Cooper pair in the BCS theory, one should immediately be alert that this potential exhibits a great promise to
open the mystery of HTSC. Here the origin of attraction between two electrons is not due to the electron-phonon interaction, instead, it is due to the correlation effects which are extremely strong at a low density of electrons and greatly enhanced by the anisotropy of the spatial structure.

Indeed, by using this marvelous potential, a series of consequences are obtained. Over one dozen of grand issues in HTSC have consistently been explained and understood.

B) A List of the Already Obtained Results

(1) The calculated critical temperature $T_C$ shows a clear dependence on doping (density of carriers), and hence the phase diagram can be reproduced as shown in Fig. 2, in which a rough bell-shape superconducting region can be seen and is basically in accord with experiment for a LaSrCuO-like cuprate.

(2) As shown in Fig. 2, the onset of the insulator-superconductor phase transition for the LaSrCuO-like compound is estimated to be $x_{is} = a^2 n_s = a^2/(2\pi c^2) \approx 0.053$ which is in excellent agreement with experimental value of \( \sim 0.05 \).

(3) The transition point where the Wigner crystallization occurs is $x_{wc} = a^2/(10\pi c^2) = 0.01$. It is also in quite good agreement with observations.

(4) $T_C$ sensitively depends on the dielectric constant of the cuprate background under investigation (Fig. 3), especially for $T_C$ over 200 K (Fig. 4). There is an optimum of $\varepsilon_k = \kappa/R$ at which $T_C$ takes the maximum.

This result leads to an understanding of the instability and difficult reproducibility of the cuprate samples with $T_C$ over 200 K (Fig. 4). This may be very helpful to those who synthesized high-$T_C$ samples and are suffering from being unable to reproduce them. For example, one happens to obtain a
sample with \( T_C \) equal to, say, 250 K in a small piece of the sample today, but one cannot reproduce it with the same equipment under the same conditions. One may even be unable to get 250 K again if one remeasures the sample after several days. Why? One is puzzled and others cast a doubt on one's discovery report. Our answer is very simple: high \( T_C \) is too sensitive to the dielectric constant to be reproduced. Although everything looks the same as before, but how can one be sure that macroscopically same conditions will result in the microscopically same defects, deformations and impurities, etc. that affect the dielectric constant? Even humidity can change the dielectric constant as well. From the guideline of \( c = 3.2 \) Å in Fig. 5, a change in \( \varepsilon_R \) by 0.6 leads to a ten-times change in \( T_C \) from 300 K to 30 K.

(5) \( T_C \) is also closely related to the interlayer spacing \( c \) (Fig. 5). Therefore, the increase of \( T_C \) under high pressure, observed by C. W. Chu et al, and the saturation of \( T_C \) at large interlayer spacing can well be explained.

(6) Moreover, the mysterious phase separation in high-\( T_C \) samples can be well understood in terms of Fig. 6, where the interlayer spacing \( c = 3.2 \) Å for a sample corresponds to \( T_C \sim 200 \) K at the piece of the sample with the doping \( x = 0.4 \) while it corresponds to an insulator \( (T_C = 0) \) for another region with \( x = 0.2 \) or smaller in the same sample. This means that inhomogeneous doping is the major cause of the phase separation.

(7) It is also easy to understand why Hg-1201 cuprate presents \( T_C = 94 \) K while the La\(_{2-x}\)Sr\(_x\)CuO\(_4\) cuprate that has a similar single-layer structure only has \( T_C \) below 40 K. From Fig. 3, a adequately small dielectric constant favors \( T_C \). Obviously, a mercury-containing cuprate is in accord with this requirement. This temperature of \( T_C = 94 \) K is likely the maximum that a single-layer cuprate may reach according to the prediction from the theory.
(8) In addition, from the theory it is possible to predict the upper limit of \( T_C \) of about 300 K for a multi-layer cuprate.

(9) It is predicted that an effect of the phase transition from a superconductor to an insulator under high pressure (Fig. 6). This may be a touchstone of the validity of the theory.

(10) No isotope effect is shown from Eq. (7). This is basically in accord with experiment near the maximum of \( T_C \). The weak and strange, in comparison with the conventional superconductivity, isotope effect can be understood with taking into account the phonon effect. But it has been found out that only near the metal-insulator (MI) transition region is its role appreciable and that its contribution to \( T_C \) is negligible in the wide region other than the MI transition.

(11) The sensitivity of \( T_C \) to \( \varepsilon_R \) is quite different for higher and lower \( T_C \), Fig. 4. This can explain why samples with lower \( T_C \), for instance, LaSrCuO cuprates, can be reproduced everywhere while higher \( T_C \) sample is almost irreducible even if it happened to be synthesized.

(12) It is not the case that any materials with a layered structure possess high \( T_C \). Note that the interelectronic coupling constant \( \alpha = \frac{e^2}{\kappa_{VF}} = \frac{R}{(\kappa a_B^0 p_F)} \), where \( a_B^0 \) is the Bohr radius and \( R = \frac{m_b}{m_e} \) with the band mass of electron \( m_b \). For example, for graphite intercalation compounds (GIC’s), \( m_b \sim 0.06 \), which leads to a very small value of \( \alpha \) and the obtained equation for \( T_C \) never yields any appreciably high \( T_C \) for this small value of \( \alpha \). A similar discussion for the materials with a large band mass, for example, strongly correlated electron systems, can show that no high \( T_C \) can be reached in these systems due to a large \( R = \frac{m_b}{m_e} \).

C) Normal State Anomalies of HTSC’s
To understand the universal anomalies of superconducting properties for cuprates (Cu-O oxides), Varma et al. made a good speculation in 1990, called the marginal Fermi liquid MFL. In terms of MFL, they could explain most of anomalies of the normal state properties. It is indeed a good success. However, the macroscopic origin of this speculation has not been clarified yet to date. Based on our model and conception, an important microscopic consequence of the FML has been obtained. It is exactly the same as speculated by Varma et al. with more details. Also, some of anomalies that could not be explained by Varma's speculation have as well been interpreted. The information regarding this is included in the paper entitled "Effects of the Vertex Correction on Charge and Spin Responses in a Layered Fermi Gas," submitted to Physica C in Jan. 1995.

This result further confirms that the model and conception used in our previous calculations are correct and the origin of HTSC indicated in our work is correct. In terms of these new consequences in the paper, the following issues can be well understood and explained.

1) Linear Dependence of In-Plane Resistivity with Temperature,
2) Nuclear Spin relaxation Time,
3) Anomalous Hall Effect,
4) Specific Heat and Thermal Conductivity,
5) Raman Scattering, etc.

III. Some Comments on the Research

(1) The comment on the Present Project
The present project has ended, but the research effort is still continued under the new support from DOE. We appreciate AFOSR for his support to initiate this exploration in superconductivity through Dr. H. Weinstock. The progress and success are faster and greater than expected. Although the previous plan to do more MD simulation on the structure of cuprates is delayed, yet more important fruitiness has obtained and makes it possible to continue in the current project of high-performance computing in superconductivity funded by DOE. The major barrier in the MD simulation - finding a proper microscopic interaction potential - has been overcome and verified to be adequate to cuprates. The simulation study is relatively earlier to be performed. Actually, eighty percent of simulational computations have been done. If the infrastructure in the scientific research at Southern University were better, it should have been completed. However, since NCSA at UIUC where the supercomputing service time was allocated updated its computing equipment in December of 1994, the CRAY supercomputer has been retired. We were unable to catch the deadline to finish all of the computations and the remaining about one-month work could not be done at all after Jan. 1, 1995 because a new supercomputing account in NCSA requires a proposal submission and application and it takes time to learn how to operate it. The SUN station computer purchased in this project in Dec. of 1994 is unable to execute all of required performances such as graphics-making, subroutine-calling, etc. The networking has just set up two weeks ago, but it still not available for use. We encountered extreme difficulty in computer-setting and using because of lacking of technical assistance. The situation is now changing towards the better direction. A baby CRAY computer seems to be soon installed in our research group through the assistance and fund from DOE.
2) Expansion of Research

We are seeking support for our effort in the mechanism of HTSC to expand our investigation to cover both theory and simulation. Also, a plan to establish a center for superconductivity at Southern for research and education is being designed and looking for funding. This center will combine theory, experiment and application (devices design) of superconductivity together. Their synergism in the same entity will promote more productive work. The concurrent education program will foster more qualified minority students for science and engineering in the next contrary.

IV. Professional Personnel

PI, J. D. Fan, Ph. D., Associate Professor, Department of Physics, Southern University, July 1, 1991 - Dec. 1994. full time in summers and 50% in the academic years.

Research Associate, Y. M. Malozovskiy, Ph. D., Department of Physics, Southern University, July 1, 1992 - Dec. 1994, full time during the whole period of employment.

Research Associate, D. S. Guo, Ph. D., Department of Physics, Southern University, Jan. 1 - June 30, 1993 (40% part time).

Research Assistant, Ping-Bo Ye, MS in physics and engineering, June 1 - Dec. 1994, full time during the whole period of employment.

V. Consultative and Advisory Functions
VI. Discoveries, Inventions and Patents

The major discovery in theory has been stated above. No tangible inventions have been made in this project. No patent. There are seven copyrighted papers.

IV. Appendixes

1) Publications under this grant.
2) Presentations during the period of this project.
1) Figures mentioned in the text.
APPENDIX 1

PUBLICATIONS
PUBLICATIONS

1992 - 1994

J. D. FAN

Department of Physics
Southern University and A&M College, Baton Rouge, LA 70813

I. Published


II. Submitted


2) Y. M. Malozovsky, J. D. Fan, "Effect of the Vertex Correction on Charge and Spin Responses of a Fermi-Liquid," PHYSICA C

APPENDIX 2

PRESENTATIONS
PRESENTATIONS

1992

J. D. Fan
Department of Physics, Southern University

I. International

None

II. National

1) Speaker, 1992 March Meeting of APS, Indianapolis, IN, Mar. 16 - 20, 1992

III. Regional & Local

1) D. S. Guo and J. D. Fan, "Energy Shift in Hydrogen Atom in a Strong Radiation Field," Fall meeting of APS TX Section, Houston, TX, Nov. 7-8, 1992,

IV. On-campus

1) Y. M. Malozovsky and J. D. Fan, "Introduction to High Temperature Superconductivity," Department of Physics, Southern University, Sep. 1992
2) G. S. Guo and J. D. Fan, "Non-Perturbative Theory of Quantum Electrodynamics," Department of Physics, Southern University, Sep. 1992
3) Z. X. Cai, Brookhaven National Laboratory, invited talk, J. D. Fan (host), "High Temperature Superconductivity and Monte carlo Simulations," Department of Physics, Southern University, June, 1992
PRESENTATIONS
1993

J. D. Fan
Department of Physics, Southern University

I. International

1) J. D. Fan and Y. M. Malozovskiy, "Electron Correlations and Superconductivity Mechanism in Cuprates," Department of Applied Physics, Chongqing University, Chongqing, China, Sep. 23, 1993


6) J. D. Fan and Y. M. Malozovskiy, "Electron Correlations and Superconductivity Mechanism in Cuprates," Hong Kong International Workshop on Computational Physics, Hong Kong, Sep. 8 - 11, 1993

7) J. D. Fan and Z. X. Cai, "Constant Temperature Molecular Dynamics (MD) Simulation Study of the Melting Transition of Rb and K in Graphite," Hong Kong International Workshop on Computational Physics, Hong Kong, Sep. 8 - 11, 1993


II. National

3) Y. Malozovsky and J. D. Fan, "Phase Transition in the System of Inter-grain Josephson Junction," 1993 March Meeting of APS, Seattle, WA, Mar. 22 - 26, 1993
4) Y. M. Malozovsky and J. D. Fan, "Boson Exchange Superconductivity in a layered Two-Dimensional Metal," 1993 March Meeting of APS, Seattle, WA, Mar. 22 - 26, 1993

III. Regional & Local


V. On-campus

1) G. S. Guo and J. D. Fan, "Earth Spin and Ozone Depletion in Stratosphere," Department of Physics, Southern University, Apr. 1993
2) J. D. Fan, "A novel Means of Information Transmission in Fiber-optical Communications Systems," Department of Electrical Engineering, Southern University, Apr. 1993,
3) J. D. Fan, "A novel Means of Information Transmission in Fiber-optical Communications Systems," Tmbuktu Academy, Southern University, Apr. 1993,
4) J. D. Fan, "A novel Means of Information Transmission in Fiber-optical Communications Systems," Department of Physics, Southern University, Mar. 1993,
PRESENTATIONS

1994

J. D. Fan
Department of Physics, Southern University

I. International & Abroad

1) Speaker, "Nonphonon Mechanism of High-Temperature Superconductivity in Cuprates," SPIE'94, Los Angeles, CA, Jan. 22 - 29, 1994
2) Speaker, "A Possible Mechanism of High-Temperature Superconductivity," Dept. of Physics, Hong Kong University of Science & Technology, June 9, 1994
3) Speaker, "A Possible Mechanism of High-Temperature Superconductivity," Dept. of Physics, Hong Kong Polytech, June 10, 1994
4) Speaker, "A Possible Mechanism of High-Temperature Superconductivity," Chongqing University, June 24, 1994

II. National

2) Speaker, "Mechanism of High-Temperature Superconductivity in a Two-Dimensional Fermi Liquid," APS 94 March Meeting, Pittsburgh, GA, Mar, 22 -26, 1994
5) Speaker, "Electron, Phonon and Plasmon: Their Roles in High-Tc Superconductivity," SESAPS annual meeting, Newport News, VA, Nov, 10 -12, 1994

III. Regional & Local

2) Speaker, "Mechanism of High-Temperature Superconductivity, "University of New Orleans, Big Muddy Quantum Fest, Feb. 10, 1994
3) Speaker, "Mechanism of High-Temperature Superconductivity," Texas Center for Superconductivity, University of Houston, Houston, TX, Mar. 2. 10, 1994
4) Speaker, "Mechanism of High-Temperature Superconductivity," Department of Physics & Atmospheric Science, Jackson State University, Jackson, MS, Apr. 7, 1994
5) Speaker, "A Possible Mechanism of High-Tc Superconductivity," Dept. of Physics, University of New Orleans, Sep. 21, 1994

IV. On-campus

1) Speaker, "Mechanism of High-Temperature Superconductivity," Department of Physics, Southern University, Baton Rouge, LA, Jan. 1994
Fig. 1. Pair interaction potential in a layered 2D system for illustrative values of the doping density $x = a^2 n_s$, where $n_s$ is the 2D density of electrons and $a = 3.8 \, \text{Å}$ is the Cu-O lattice constant; and the interplanar spacing $c = 6.6 \, \text{Å}$ and the effective Bohr radius $a_B = 1.0 \, \text{Å}$.

(a) in-plane potential. (b) potential in the direction normal to the plane.
Fig. 2. Transition temperature $RT_c$ and the renormalization factor $Z(0)$ vs. the doping density $x$ for LaSrCuO; where $R = m_b/m_o$, $m_b$ is the band mass of electron. The use of interlayer spacing $c = 6.6$ Å and the lattice constant $a = 3.8$ Å was made to fit the maximum $T_c \sim 37$ K.

Fig. 3. Variation of the transition temperature $RT_c$ with $\varepsilon_r = \kappa/R$ at $x = 0.15$; where $R = m_b/m_o$, $m_b$ is the band mass; $\kappa$ is the dielectric constant of a single-layer cuprate; given interlayer spacing $c$ as parameters. Note there exists a maximum $RT_c \sim 95$ K at $\varepsilon_r \sim 2$ and $c \sim 4$ Å.
Fig. 4. Comparison of the transition temperatures $RT_c$ vs. $\epsilon_R = \kappa/R$ at the optimum doping; where $R = m_b/m_e$, $m_b$ is the band mass; $\kappa$ is the dielectric constant of cuprate. Note the rapid drop of $T_c$ with $\epsilon_R$ deviation from the optimum for the room-temperature superconductivity.
Fig. 5. Variation of the transition temperature RT\textsubscript{C} with the interlayer spacing, given $x = 0.99$, for an infinite-layer cuprate; where $R = m_b/m_e$, $m_b$ is the band mass of electron. Note that $T_C$ changes drastically with $\varepsilon_R$. An increase of $T_C$ with decreasing $c$ and a saturation of $T_C$ at the large interlayer spacing are shown.

Fig. 6. Variation of the transition temperature RT\textsubscript{C} with the interlayer spacing $c$, given $\varepsilon_R = \kappa/R = 1.1$, for an infinite-layer cuprate; where $R = m_b/m_e$, $m_b$ is the band mass of electron. There exists a cutoff spacing $c_{\text{cut}} \sim 2.3$ Å at $x = 0.4$ or $c_{\text{cut}} = 3.3$ Å at $x = 0.2$. A saturation of $T_C$ at the large interlayer spacing appears.